MODELING TRANSPORT PHENOMENA IN THE DRYING PROCESS OF FERMENTED CACAO BEANS

By

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This dissertation is dedicated to my beloved wife, Ana Maria,
and children, Guga, Guga, and Vivi with affection

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KEY TO SYMBOLS

a_w	water activity, decimal
A	acetic acid mass ratio, decimal
B_x	element volume interface area perpendicular to the x direction
B_y	element volume interface area perpendicular to the y direction
B_z	element volume interface area perpendicular to the z direction
c_p	specific heat capacity, J/kg °C
C	mass concentration, kg/m³
d	bean thickness, m
D	mass diffusivity, m²/s
e	specific internal energy, J/m³
h_c	convective heat transfer coefficient, W/m² °C
h_m	convective mass transfer coefficient, kg/m² s
H_{fg}	latent heat of vaporization, J/kg
I	rate of mass production or consumption due to phase change, kg/m³ s
j	Chilton-Colburn j-factor
J	generalized flux vector through unit area
K_{ij}	generalized transfer coefficients

k	thermal conductivity, W/m °C
l	bean length, m
L_{ij}	generalized phenomenological coefficients
m	mass, kg
$\mathbf{n}$	outward-directed normal unit vector
Pr	Prandtl number
q	heat flow, W
R	ideal gas constant, m^3 Pa/kg °K
Re	Reynolds number
Sc	Schmidt number
t	time, s
T	temperature, °C
$\mathbf{v}$	velocity vector, m/s
V	volume, m^3
w	bean width, m
W	dry basis moisture content, decimal
x	distance in the x direction, m
$\mathbf{x}$	position vector
y	distance in the y direction, m
Y	air humidity ratio, decimal
z	distance in the z direction, m

Greek symbols

ξ_i	outward-directed normal unit vector
ρ	mass density or concentration, kg/m^3
ρ_b	density of bone-dry material, kg/m^3

Superscripts

t	time

Subscripts

a	acetic acid
c	heat convection
i	index for the x direction
j	index for the y direction
k	index for the z direction
l	liquid phase
q	heat
0	initial conditions or free state
s	solids
v	vapor phase
w	moisture
∞	drying air (bulk stream)

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Cacao is a tropical crop well known for its end product, the chocolate. Before reaching this point, the fresh seeds have to be cured on the farms. Curing involves fermentation and drying, which are essential processes to the development of the chocolate characteristic flavor and color, later, in the manufacturing stages.

The transfer mechanisms related to the drying of cacao beans are little understood and studied. Most of the research carried out up to now has focused on large scale drying tests and adaptation of dryers used for other products. As a consequence, many farm processing systems have low efficiency and do not yield a competitive product. To achieve higher efficiencies in processing operations, there is need for developing simulation models to predict transport phenomena in the drying of cacao that take as inputs the physical properties inherent to the product.

A mathematical model, based on the theories of heat and mass diffusion, was derived and used to simulate the drying of fully exposed cacao beans. The model consisted of four partial differential equations to describe the transfer of solids due to shrinkage, energy, moisture and acetic acid produced during fermentation. This model was also used to determine a regression model for mass diffusivity from drying data as a function of product temperature and moisture. A computer program was implemented to solve the model equations numerically. The control volume approach was used to derive the difference equations which were solved by the explicit finite difference method.

Experimental tests were designed to determine moisture diffusivity in cacao and to validate the model in the temperature and airflow ranges normally used to dry the product. The drying air temperatures varied from 40 to 70 °C, while air velocities were in the range of 0.1 to 2.5 m/s.

Good predictions of average moisture content were obtained with the model. However, it was not possible to drive off perceptible quantities of acetic acid by drying cacao at temperatures up to 80 °C. Therefore, in this respect, artificial drying may not contribute to improve the quality of cacao with high acetic acid concentrations.

CHAPTER 1
INTRODUCTION

Statement of the Problem

Cacao is a cash crop and the major source of revenue for many producing countries. This has contributed to the large production increases in world production during the past few decades. Global production of dry beans has doubled since 1960 (Table 1.1) and reached the record of 2.4 million tons in 1992/93 (Wakeling, 1994). Area expansion and new plantings in some countries were the principal reason, rather than increase in productivity and efficiency (Smith, 1994). This factor and the low elasticity of the product demand have led to a depression in the international market prices. With the current situation the market is more competitive, particularly for those producers that had to modernize farming systems to cope with the need for larger drying capacities and quality amelioration.

Use of new technologies and innovation involved significant capital investments and contributed to the total production cost escalation. This is the case for some Asian and South American countries as opposed to those in West Africa. African production systems are typically low input, low-output and low-technology systems (Lass, 1993). Latin American countries have the highest total producing costs. The costs for processing

raw cacao on the farm follow the same trend and are comparable to those of Asian countries (Bloomfield, 1994)

Table 1.1. Evolution of world cacao bean production (x 1000 metric tons) (*Source* International Cocoa Organization - ICCO, 1993)

Year	1960	1970	1980	1990
Production	1046	1416	1632	2207

Brazilian cacao, in particular, has other problems associated with quality Chocolate manufacturers are strict on their requirements They need cacao that can be processed into chocolate with natural flavor (Powell, 1981) Some have claimed that Bahian cacao has some undesirable flavors such as contamination by smoke and excess acidity The greatest consuming countries in Europe impose severe constraints on Bahian cacao to the point of not importing any from Brazil American manufacturers also impose some restrictions The maximum amount of Bahian cacao included in their blends is between 20 and 25% (Table 1.2) It is alleged that anything higher than that would alter their product flavors and reduce sales (Schwan, 1984)

There has been a great deal of research effort to apply engineering knowledge to drying of fermented cacao Studies and improvement of existing drying facilities have been done in Brazil (McDonald and Freire, 1981, 1982, McDonald et al., 1980, Cunha, 1991). Work to adapt drying equipment used for other grains and to develop new

dryers for cacao has also been done (Ghosh, 1972a, 1973a, Freire et al , 1984, Cunha, 1984).

Table 1 2 Major cacao bean consumers and Brazilian imports in 1991/1992 (*Source* International Cocoa Organization - ICCO, 1993)

Country	Consumption		Brazilian imports	
	Per caput (kg)	Total (t)	(t)	(%)
Belgium	5.516	46.900 00	0 00	0 00
Switzerland	4 821	34 600 00	0 32	0 93
Germany	3.279	277 000 00	6.15	2 71
England	3 118	182,600 00	7.67	4.20
France	2 785	156 400 00	0 00	0 00
Netherlands	2 488	36 200 00	9 92	27 40
United States	2 327	566,200 00	139 04	24 56
Canada	1 796	46 600 00	11 66	25 02
Italy	1.289	70 800 00	0 00	0 00
Japan	0 891	109 300 00	10 16	9.30

Despite these efforts, there is need to develop research in this area as a means of better understanding the process and obtaining more reliable information about drying of cacao The drying behavior of a material depends on its physical properties, and very little attention has been paid to the intrinsic characteristics of cacao beans with respect to their drying

It is necessary to face the urgency of the situation and the scarce resources available for research. Field investigations are laborious, time consuming and expensive (Singh et al , 1993) With precise engineering modeling, it may be possible to design efficient, cost effective drying systems and sound procedures for processing raw cacao Therefore, there is great demand for using more rational approaches to the problem. This involves the use of tools such as mathematical modeling, simulation and optimization techniques. Computer simulation has proved to be useful in giving insight into the physics of transfer processes (Parti, 1990) The availability of powerful and cheap microcomputers makes their use readily feasible The final goal is to obtain a more competitive product in terms of both production costs and quality improvement.

Project Objectives

The global objective of this research project was to simulate the drying process of fermented cacao beans under conditions of fully exposed beans or thin layer drying. The following were the major specific aims

1 Develop a mathematical model to describe the simultaneous phenomena of mass and heat transfer involved in cacao drying.

2 Determine the effective mass diffusion coefficients for fermented cacao beans.

3 Validate the simulation model under the conditions with which cacao is normally dried.

CHAPTER 2
CACAO PROCESSING

The Swedish naturalist Carolus Linnaeus (1707-1778) named the species as *Theobroma cacao* Theobroma is the Greek equivalent for "food of the gods" (De Zaan, 1974) The current literature suggests the use of the word cacao to refer to the species and the crop itself whereas the term cocoa should be used for the powder (Wood and Lass, 1985) a product obtained at the grinding and manufacturing plants This expression, however, finds more common and frequent use in the commercial milieu and everyday life

Origin and Distribution of Cacao

This species and several others of the same genus, which are of inexpressive or no commercial importance, seem to have their origin in the Amazonian region, a center of diversity, where a great populational variation may be found (Wood and Lass, 1985). According to the most accepted theories, two major groups originated from the lower Amazon river basin through the process of natural evolution (Smith, 1994) Figure 2.1 depicts the origin and migration of cacao to the major producing regions in the world

Figure 2-1. Center of origin and evolution of cacao and other species of the genus *Theobroma* (*Source* Adapted from CEPLAC, 1982)

One group is known as Criollo cacao It is denoted in the international market as fine flavor cocoa. The reason for this lies in the fact that this type of cacao has a much stronger bouquet and distinctive flavors (Williamson, 1985) The varieties that belong to this group are presently grown in small areas of some countries in Central America, Caribbean islands, Far East Asia and in some Pacific islands

The crop itself is very susceptible to plant diseases and it is more strogeot io terms of cultivation requiremeots. Its partiepatioo in the total world production is not very significant, however It may comprise less than 10% of the whole volume traded yearly in the international market. The trend is for fioe cocoas to disappear, as predicted by some specialists (Powell, 19$1)

The secood group is usually known as Frrastero cacao or bulk cocoa in the commercial jargon. This kind of cacao has a weaker chocolate flavor and makes up the bulk of the product marketed in the world (Wood and Lass 1985) It is grown in some countries of the American, African and Asian continents, in the so-called cocoa bean belt (Godtva, Undated) This region encompasses the tropical belt, a range around the globe within 22 degrees of latitude north and south of the equator line (Figure 2.2). Ivory Coast and Brazil are the leaders in the rank of producing countries accounting for nearly half of the world s production. About 90% of the Brazilian production comes from the southern parts of Bahia State hence, the expression Bahian cocoa used in international transactions

These two groups present some major differences in the characteristics of their seeds Forastero cacao has cotyledons of purple color due to the presence of anthocyanins It also takes more time to be fully fermeoted The Criollo cacao, on the other hand, has seeds with white or light color interior Its fermentation requires a very short time, oearly half or less of that required by Forastero cacao (Lopez, 1986) The time required for full development of chocolate flavor during roasting is also comparatively shorter

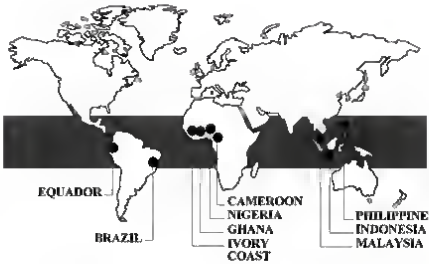


Figure 2.2. Major cacao producing countries.
(*Source* adapted from CEPLAC, 1984)

Crosses between specimens of these two major types produced a third type known as Trinatario cacao. This is a very heterogeneous group and its supply in the market is intermediate between the other two groups (Lehman and Patterson, 1983).

Harvest and Processing of Raw Cacao

Harvest of cacao consists of removing ripe and partially ripe pods from the trees. The fruits are then gathered in convenient sites in the field or transported to the fermentaries for the task of pod opening and extraction of the seeds. The frequency with

which the fruits are collected varies markedly from region to region (Jones and Jones, 1984) and with the season.

The time between harvest and seed extraction may also vary. Pod storage for periods of up to 12 days, with other related practices, are recommended in some producing areas for crop conditioning. This procedure helps to achieve better quality by diminishing subsequent acid formation during the curing process (Duncan et al., 1989, Alamsy, 1991). Reduction of the bean total acidity enhances chocolate flavor in the end product (Liau, 1978). Weaker flavor has been found in chocolate prepared from cacao with pH values less than 4.5. The converse has been verified for samples with pH values above 5.0 (Biel et al., 1989). However, where the weather is very humid and hot, pod storage may not be feasible due to mold development and rapid product decay. Furthermore, conditioning does not always yield the expected outcomes (Dias and Avila, 1990).

Raw cacao has to be processed or cured before it can be marketed. Curing is normally done on the farms. The fresh seeds have a moisture content approximately 60% wet basis (Passos and Passos, 1989). In addition, the seed coat has an outer layer made of a mucilaginous and sticky pulp. These peculiarities make handling of the fresh material a difficult operation. The raw product is quite unsuitable for long distance shipping and storage.

Curing involves two major practices: fermentation and subsequent drying. Both are equally important to the quality of the product (Lopez, 1986).

Cacao Fermentation

The term fermentation is commonly used to describe the physical and chemical changes, which occur in the preparation of the beans before drying. It is considered as a misleading expression by some specialists. Curing has been suggested to provide a more comprehensive picture of the process (Knapp, 1937, Forsyth and Quesnel, 1963, McDonald et al – 1981). This is to reflect physical and chemical complexities of the process, the variety of agents responsible for them, and the association with the drying process.

Microbial or true fermentation takes place in the process, but most important are the subsequent chain of biochemical changes inside the beans. Development of chocolate flavor potential in the product strongly depends on them (Lopez, 1986). Unfermented cacao develops no characteristic chocolate flavor whatsoever, if dried and roasted.

The simplified diagram shown in Figure 2.3 illustrates the chemical changes of cacao fermentation. It is based on data found in several review and technical papers published on the subject. It is important to stress, however, that the fermentation stages are not clear cut, there is considerable overlaps among them.

The pulp that surrounds the cacao seed may account for up to 40% of its weight and nearly 90% of the pulp is water (Freire et al , 1990). It contains an average of about 14% of fermentable sugars. Sucrose is the predominant sugar and its concentration may achieve levels up to 60% of the total sugar content (Berbert, 1979). The pulp is quite acid,

pH value around 3 5, due to the presence of citric acid. The pulp makes up an adequate substrate for the growth of several categories of microorganisms

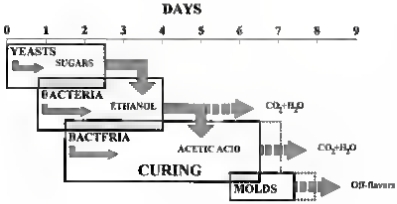


Figure 2.3 Schematic representation of cacao fermentation, principal agents involved in the different stages and resulting metabolic products

Batch fermentation is the most common method used in Brazil. It consists of fermenting the product in wooden containers subdivided into two or more compartments Each compartment has a volumetric capacity of 1 2 m^3 The average output of one compartment varies between 850 and 950 kg of fermented beans This process may take from five to seven days (Freire et al., 1992).

The mass of cacao in each compartment of the fermentor is turned over and mixed at least once every other day in the course of the process Turning helps promoting aeration (Schwan et al , 1990), and uniformity of the mass undergoing fermentation.

The physical characteristics of the pulp at the beginning of the process help to form a medium of low oxygen tension in the fermentor The prevailing conditions and the rich substrate allow the proliferation and dominance of yeasts at first. This group of microorganisms metabolizes fermentable sugars into ethanol and carbon dioxide (Vincent and Galzy, 1983) Higher levels of CO_2, lower acidity and moderate temperature elevation favor the growth of lactic acid bacteria. Production of lactic acid takes place to a greater or lesser extent, depending on the maintenance of adequate conditions

Simultaneously, the breakdown of the pulp cells, fibers, pectin and other components occurs, helping the drainage of the liquid pulp through the mass of beans This promotes increasing aeration, which is further enhanced by turning the product Modifications in the conditions of the medium occur continuously and induce changes in the type of population of microorganisms that predominates Eventually acetic acid bacteria prevail over the yeasts and oxidize alcohol into acetic acid, which is further broken down into CO_2 and water This sequence of reactions involving microorganisms generates enough heat to raise the product temperature well above the ambient. The temperature of a batch under fermentation may achieve values up to 56 °C (Schwan, 1984)

Acetic acid is the major volatile acid present in fully fermented Brazilian cacao Its concentration after six days of fermentation is about 1.5% (Lopez, 1983) Diffusion of

acetic acid into the cotyledons leads to seed death (Quesnel, 1965). The consequences are the loss of internal compartmentation, prevention of butter degradation by reactions in the germination process, and disintegration of the surrounding pulp. Lack of cellular integrity increases permeability among the cells. This allows better contact between enzymes and substrates (Lehrian and Patterson, 1983), and triggers a chain of complex and extremely important biochemical reactions responsible for the formation of compounds generally known as precursors of chocolate flavor.

The beans experience a concomitant and steady change of color, due to enzymatic oxidation, which is responsible for the production of brown pigments. This effect has auxiliary importance in the composition of chocolate flavor precursors. Moreover, use of color change to monitor and decide when the process ends is a very common practice. After a period of five to seven days, a sharp brown ring appears around the cotyledons. It can be easily seen when the bean is cut open. Color is also used for assessing the quality of dry cacao through the so-called cut test. Despite its common use in cacao transactions, it has severe limitations for evaluating the potential of chocolate in a sample (Lopez and McDonald, 1981).

Overfermentation can cause harm to the product. Higher oxygen tension and lower acidity are the normal conditions at the end of the process. The medium temperature is still high, therefore; the growth of spore forming bacteria occurs (Schwan, 1984). They may dominate the medium if the mass of cacao remains in the fermenting box over time. This group of microorganisms produces substances responsible for some off-flavors in the chocolate. Excessively long fermentations cause putrefaction

of the pulp and skin and development of objectionable flavors (Forsyth and Quesnel, 1963) Molds and fungi other than yeasts, may also grow and further spoil the product They present the greatest problem during drying (Lopez, 1986)

Drying of Cacao

Drying of the beans should start soon after completion of the fermentation process to avoid deterioration of the wet product. The initial moisture of fermented cacao varies between 50 and 55% wet basis depending on region, variety and season (Ghosh and Cunha, 1975, McDonald and Freire, 1981) Drying must bring moisture down to 7 to 8% for safe storage (Gramacho et al , 1992) This results in the removal of large quantities of water, roughly equivalent to half of the freshly fermented bean weight Fermentation makes drying easier the pulp decay increases the permeability of the bean shell Even so cacao drying is an energy intensive process

One should not consider drying of cacao as a matter of water extraction only It requires extra care not normally required for other agricultural products Progression of the oxidative reactions accounts for the development of the characteristic chocolate brown color and reduction of bitterness and astringent flavor (McDonald et al 1981) Drying in this context should be regarded as an integral part of the curing process since it contributes to the improvement of cacao intrinsic qualities

Sun drying is the most common method used in many countries (McDonald et al., 1981) In Brazil, in particular, it is carried out on flat wooden platforms with sliding roofs to protect the beans at night and during rains (Ghosh and Cunha, 1975). The drying

area of these platforms varies from 6 m^2 in small holdings, to 72 m^2 in large plantations (Freire et al., 1992). Natural drying is strongly dependent on weather conditions. Its duration may take from 7 to 20 days for completion. Weather permitting, it has some advantages. It is a slow process, therefore, it allows for a smooth continuation of the curing reactions and their completion to the desired level. On the other hand, the product may be spoiled under bad weather conditions. Low output per unit area and need for regular stirring are also major drawbacks to its use (McDonald et al., 1981). Very often drying has to be finished with the aid of heated air. Artificial drying is especially essential in growing areas where the rainy season coincides with the cacao harvest.

In artificial drying the product is subjected to a stream of hot air. Either natural or forced convection are used to force air through a static bed of beans (McDonald and Freire, 1981). In both cases, indirect heating of the drying air is indispensable to avoid contamination of cacao with products of combustion (McDonald and Freire, 1982). Dried cacao has a butter content up to 57% (Ribeiro, 1988), it is prone to off-flavor uptake. Smoky flavor was a major constraint imposed on Brazilian cocoa in the past (Berbert and Lopez, 1979). Simple modifications in the traditional drying facilities have remarkably contributed to the solution of this problem (McDonald et al., 1980).

There is a consensus in the literature that the temperature of the product should not reach values much higher than 60 °C before the desired level of browning is attained. Very high temperatures may inactivate the enzymes involved in biochemical changes.

Cacao Grinding and Chocolate Manufacturing

After drying the product may be stored before marketing. Farm storage is usually done for very short periods of time, no more than three months. The dried beans are ready to be processed into liquor or chocolate. Figure 2.4 illustrates the basic operations carried out in the processes of grinding: production of cacao butter, powder and liquor or plain cacao mass and manufacturing of plain chocolate. In some plants the whole beans are roasted just after cleaning, then they are cracked and winnowed.

Roasting is one of the most important stages of chocolate manufacturing since it is in this process that chocolate flavors are formed. During roasting the beans are heated to temperatures between 100 and 120 °C for about 45 to 70 minutes (Wood and Lass, 1985).

Most of the terms used in the diagram are self-explanatory. The word nib refer to the pieces of cotyledons obtained after a coarse grinding. The expression liquor is used to designate the mass of cacao finely ground. The liquor has an average butter content close to 53% (Cook, 1972). The amount of butter in the powder varies according to its end-use and manufacturer. High fat powders, containing 22 to 25% of butter, are used for cocoa based drinks; while low fat powders (10 to 13%) are used as food flavoring (Wood and Lass, 1985).

Plain chocolate may be obtained from the liquor by addition of butter and sugar. Additional treatments of the mixture, such as conching and tempering, are required to enhance the chocolate flavor.

Conching is a practice that consists of subjecting the chocolate paste to a controlled thermal treatment and agitation combined with mechanical aeration. The results are flavor improvement due to increase in smoothness, elimination of some undesirable volatiles and controlled oxidation (Cook, 1972). Tempering consists of controlling the cooling the chocolate mass to avoid formation of butter crystals.

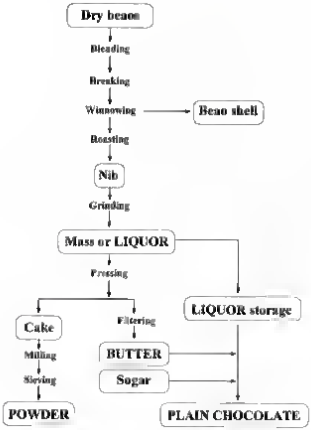


Figure 2.4 Flowdiagram of cacao grinding, production of butter, powder, liquor and plain chocolate

Alkalization is another method used to control excess acidity of some cacao. This is a thermal process that consists of treating the nibs or liquor with an alkali solution. It can be tuned to produce cocoa powder of a diversity of colors in the brown scale to suit the consumer's needs (De Zaan 1974). This treatment was first devised as a tool to improve quality of those cacaos characterized as acidic in the market. However, the "Dutch process", as it is known, does not lead to improvement or strengthening of flavor. On the contrary, it has the same effect as excess acidity, that is, it tends to weaken the chocolate flavor of the untreated product (Cook, 1972).

Chocolate is the principal product derived from fermented cacao. Yet cacao finds countless uses in many branches of the food, chemical, pharmaceutical and cosmetic industries.

CHAPTER 3
LITERATURE REVIEW

Drying is an old activity (Hall 1990). Man has been using it to preserve his primary food provisions since the primordial era by exposing them to the sun and wind (Keey, 1980). This practice has undergone considerable development over the years. Nowadays it is employed as a convenient means of preparing agricultural and animal products for storage and marketing. The process of drying is one of the most energy intensive operations (Strumillo and Lopez-Cacicedo, 1987). However, it can be made simple and cheap compared to other forms of food preservation. Efficient equipment is available, as a result of effective process design, which can be used with success.

The drying operation consists of extracting moisture from the associated material by supplying energy to it. A convection medium, hot air, is commonly used to heat the product, and to carry away the moisture driven off from the material. In fact, the term drying applies to the removal of volatile substances from a solid material through heating (Keey, 1972, Menon and Mujumdar, 1987).

Drying Theories Used for Grains and Foods

Water migration in hygroscopic materials may be described by many physical mechanisms as proposed in the literature (van Arsdel, 1963, Fortes and Okos, 1980, Strumillo and Kudra, 1986, Brooker et al 1992)

1. Liquid migration due to capillary suction or gradients in capillary pressure
2. Liquid diffusion due to moisture concentration gradients inside the material
3. Diffusion of layers of liquid adsorbed on the pore walls due to gradients at these surfaces
4. The evaporation-condensation mechanism in partially filled pores due to partial pressure gradients.
5. Vapor transfer due to gradients in total pressure occurs when the material achieves temperatures well above the boiling point
6. Mass flow due to thermal gradients in the medium known as thermal diffusion.
7. Liquid flow in porous materials due to gravitational and centrifugal forces
8. Effusion flow or Knudsen diffusion when the pore diameter is of the order of the mean free paths of the vapor molecules.
9. Transport owing to osmotic pressure This type of pressure is a function of the moisture gradient in the medium.

Drying simulation models may be classified according to their capability of coping with one or more of the mechanisms of moisture migration (Rossen and Hayakawa, 1977)

They may occur either independently or simultaneously during drying, depending on the conditions and product.

Extensive reviews of the uses, development and advances in the theoretical foundations of drying kinetics are presented in Mujumdar (1980). They reveal most of the developments and investigations on the use of empirical, semi-empirical and theoretical models. Empirical models do not allow for any aspects of the basic principles of conservation to make predictions about the transfer of mass and energy (Parti, 1990). Their uses, therefore, are restricted to the material and conditions for which they were developed (Fulford, 1969). Theoretical models are founded on the principles of momentum, mass and energy conservation. Basically, the approach to drying theory consists of establishing a set of partial differential equations of heat and mass transfer with phase change (Martynenko et al., 1980). They may be complemented with the concepts of interactive fluxes of the thermodynamics of irreversible processes (Fortes, et al., 1981).

The mathematical treatment of these models is considerably involved (Furuta and Hayakawa, 1992), and especially difficult to validate (Litchfield and Okos, 1992). Besides, the mass transfer coefficients are not amenable to direct measurement in all cases. This is so because drying comprises highly complex interactions between heat and mass transfer. In addition, several simultaneous mechanisms by which moisture migrates within the material may be present (Fulford, 1969). In many situations, the transfer coefficients for the different mechanisms are lumped together or one may be considered as overriding the others. This is usually done for practical reasons, resulting in semi-

empirical models that are more tractable. Semi-empirical models are used in situations where the present state of knowledge and the complexity of the process do not permit a formulation of the problem based solely on theoretical arguments.

Moisture transfer, either in the form of liquid or vapor transport, may be used for describing moisture movement during drying. This is represented by Equation 3.1 for transfer under transient regime (Crank, 1975). Although this is not universally accepted, it seems to be the approach most used for simulating drying behavior of foods and grains.

$$\frac{\partial M}{\partial t} = \nabla.(D\nabla M) \qquad \textbf{(3.1)}$$

where M = moisture concentration
t = time
D = moisture diffusivity

Analytical solution of this partial differential equation with different types of boundary conditions may be expressed in terms of infinite series for bodies of regular geometries (Crank, 1975, Mikhailov and Ozisik, 1984). Usually the solution used in drying simulation is for prescribed or imposed boundary conditions and the supposition of a constant diffusion coefficient.

Diffusion appears to be the most agreed upon controlling mechanism (Hutchinson and Otten 1983, Parry, 1985, Parti and Dugmanics, 1990, Sun and Woods, 1994). Isothermal conditions within the product are assumed. When both vapor and liquid migrations are present, the diffusion coefficient represents the combined effect of both mechanisms and may be considered as an effective coefficient.

Drying theories as applied to agricultural crops and foods consist of treating the process of heat and mass transfer as a two-component system. This may be a reasonable approach for some materials, where the drying mechanism involves exclusively heat transfer and moisture migration. In most practical situations water is the major constituent of moisture and the only concern. For example, the major function of grain drying is to remove excess water to control the growth of microorganisms.

With other products, however, volatile compounds should be considered. These substances usually play an important role in the organoleptic characteristics of the product. Sometimes losses of desirable compounds are deleterious, whereas in other cases it is required to remove undesirable substances to levels acceptable for consumption, depending on the end use of the product.

Acetic acid produced during fermentation and curing of cacao is one of the components that have to be reduced to desired levels. It seems that acetic acid degradation inside the beans under fermentation is not representative (Lehrian and Patterson, 1983). Part of it is lost in this stage and in the drying process, as well as during the further stages of chocolate manufacturing.

Keey (1972) suggested the use of the multicomponent diffusion theory for dealing with this kind of situation. This procedure consists of deriving a separate continuity equation for each mass species in the system. Whence, it leads to a set of coupled partial differential equations of the form:

$$\frac{\partial C_i}{\partial t} = \sum_{j=1}^{n-1} D_{ij} \nabla^2 C_j \qquad \textbf{(3.2)}$$

where C_i = concentration of species i
t = time
D_{ij} = diffusivities and cross diffusivities.

Because of the correspondence between mass diffusion and heat transfer by conduction in solids, both processes may be treated similarly. Therefore, energy may be regarded as another species and included into the system of equations above to avoid its isothermal constraint.

Drying Theories and Related Topics as Applied to Cacao Beans

Several reviews and technical papers on drying of cacao can be found in the literature. All the reviews give good account of the process and related topics, the many types of driers in use in different countries (McDonald et al., 1981; Wood and Lass, 1985), and in Brazil (Cunha and Serodio, 1991). The major engineering problems of equipment design, adaptation for cacao and improvement of thermal efficiency are also dealt with (Ghosh, 1972b, Cunha, 1991). An important aspect of the subject is the relation between the engineering and biochemical facets of the process (McDonald et al , 1981).

Most of the research work carried out on cacao drying was concerned with field drying experimentation. Several types of driers were tested with special regard to thermal performance, effect of different drying schemes on the product quality and operational costs. Lumped energy and mass balances were used to develop simple mathematical expressions to calculate coefficients of global efficiency for drying systems. Usually

these coefficients grouped together the efficiencies of fuel combustion, heat exchange and efficiency of the drying process itself.

McDonald et al (1981, p 19) proposed the use of the overall drying efficiency (Equation 3.3) to make comparisons among different kinds of drying systems. The definition of this coefficient is given as "that proportion of the energy liberated at the combustion stage which is actually used for the evaporation of moisture with the remaining proportion representing lost heat." Although care is recommended when employing this coefficient, the authors state that it can be useful for comparing different drying systems running under similar conditions. The latent heat of moisture vaporization is assumed constant and equal to that of boiling free water.

$$\nu = \frac{WL}{FC} \tag{3.3}$$

where ν = coefficient of overall efficiency (dimensionless)
W = amount of water evaporated in the process (kg)
L = latent heat of vaporization of water (J/kg)
F = mass of fuel used (kg)
C = combustion heat of the fuel (J/kg)

An exception to this type of approach was presented by Bravo and McGaw (1973). These researchers investigated the behavior of cacao during drying in packed beds at the maximum temperature recommended in the literature, approximately 65 °C. Regression procedures were used to find the relationship between the time to dry the product to a moisture of 6.4% (dry basis) and its initial moisture content, airflow rate and bed depth (Equation 3.4). The model was further used to optimize costs of drying

schemes This approach may be considered an improvement over what had been done so far

$$\theta = \frac{(X_o - 0.3)}{\exp(-2.8482 + 0.0277U - 0.1154H)} + 22 \qquad (3.4)$$

where θ = time required to dry the product to 6.4% dry basis (hour)
X_o = initial moisture content (decimal, dry basis)
U = air velocity (ft/min)
H = height of the static bed of cacao (inches)

Many important viewpoints of cacao drying are discussed in a review by McDonald et al (1981) This paper covers a broad area of field research on cacao drying and quality of the product. Theoretical aspects that pertain to cacao itself are examined in purely descriptive terms Some topics considered are the relation between heat and moisture transfer and acetic acid evaporation, and the interface between this process and fermentation Loss of acetic acid during drying seems to be a controversial matter Some researchers believe that considerable amounts of this acid can be driven off during drying whereas others are skeptical about this possibility and state that these losses are derived entirely from the exterior of the bean The rate of moisture removal is high enough to not allow for sufficient time for acid diffusion and evaporation

Bravo and McGaw (1974) seem be the first researchers to carry out a study on the fundamentals of the drying of cacao They investigated drying of fully exposed beans under controlled air conditions and gave a mathematical interpretation to the drying curves The range of airflow rates and temperatures used were between 0.05 and 1.29 m/s and 37 to 86 °C, respectively In this work, three distinct drying periods were

observed Logarithms nf the slopes of these portions of the moisture loss curves were empirically correlated to the drying air conditions such as temperature and airflow rate (Equations 3 5, 3 6 and 3 7, respectively) The first period, the constant rate period, was given as a function nf air velocity and temperature, whereas the last two depended on the drying air temperature only

$$\ln\left(-\frac{dX}{d\theta}\right) = -2\,48 + 0.025T + 0\,0186U \tag{3.5}$$

$$-\frac{d(\ln X)}{d\theta} = 0\,00565T + 0.144 \tag{3.6}$$

$$-\frac{d(\ln X)}{d\theta} = 0\,003T + 0.0075 \tag{3 7}$$

where X = product moisture content (decimal dry basis)
θ = drying time (hours)
T = air temperature (°C)
U = air velocity (m/min)

Analog of Newton s law of cooling has also been used to describe the intrinsic drying behavior of cacao in thin layers An expression for thin layer drying may be obtained by analogy to transient heat conduction of a lumped mass subjected to forced convection (Equation 3.8) The primary and important assumption is that the material itself nffers negligible resistance to mass transport. The actual resistance to moisture transfer is distributed across the film envelnping the body (Sisson and Pitts, 1972, Keith and Black, 1980 Ineropera and Dewitt 1990) It is sometimes called the exponential or logarithm model in the drying literature (Brooker et al., 1992)

$$MR = \frac{M - M_e}{M_o - M_e} = \exp(-kt) \qquad (3\ 8)$$

where MR = moisture ratio
M = actual product moisture
M_e = equilibrium moisture content
M_o = initial moisture content
k = drying constant of the material
t = drying time.

The equilibrium moisture content (M_e) may be defined as the amount of moisture present in the product when its internal vapor pressure equals that of the environment to which it is exposed This parameter dictates the extent to which a material can be dried under a specified state of the drying air (Keey, 1972 Strumillo and Kudra, 1986 Brooker et al , 1992)

The expression above resembles the analytical solution of Equation 3 1 for prescribed boundary conditions if the series is truncated after the first term According to Sun and Woods (1994) Equation 3 8 has a strong theoretical foundation, since it represents the first term of the infinite series If this was so, then the drying constant would represent the internal resistance to moisture transport This contradicts the basic assumption behind Newton's law of cooling, which is the lack of internal resistance to moisture transfer

Similar model was used for cacao under different drying air temperatures (Cunha, 1983) Two major drying periods were observed The first was characterized by a constant drying rate that can be more appropriately described by means of analogies to the Newton s law of cooling The second stage was characterized by a falling rate

behavior, suggesting a change in the type of resistance to moisture transfer. Despite the relatively high amount of free moisture in fermented cacao, only one airflow rate of about 0.15 m/s, based on suggestions available in the cacao literature for drying under field conditions (Shelton, 1967; Wood, 1971), was used to obtain this model. Introduction of extra parameters into the Newton's law improves curve fit for cacao as reported by Sasseron (1984). This is expected, since it is always possible to obtain better fit of a model to a set of experimental data by adding new regressand constants in the model (Jayas et al., 1991).

Although it has been possible to achieve good agreement between experimental and simulated data, these models do not consider some aspects inherent to cacao beans. Some peculiarities of cacao are the size of the beans and the large volume shrinkage that occurs during the drying process. Cacao beans are much larger than common grains. Typical length, width and thickness for freshly fermented beans are 24.39, 13.08 and 8.81 mm, respectively (Ghosh, 1973b, 1976). These characteristics vary considerably with variety, however. Reduction in bulk volume of cacao during drying may be as high as 30% of the initial volume (Cunha et al., 1983). Shrinkage has considerable effect on the response of simultaneous heat and mass transfer models used for drying simulation of foods (Balaban, 1989).

The literature reviewed confirms that very little is known about the drying behavior of cacao. The models used may fit specific experimental data well, but their use cannot be generalized. None of them takes into account the special characteristics of cacao beans.

CHAPTER 4
MATHEMATICAL MODEL

Mathematical modeling is a powerful tool for formulating engineering problems in terms of sound mathematical statements so that prediction of future events can be made possible. Nevertheless, a model is a compromise between the complexity of the physical phenomena and the capability of solving the problem, either analytically or numerically (Stanislav, 1982).

A model for simulating transport phenomena in the drying of a material should be as complete as possible in order to give in-depth insight into the actual phenomena that take place during the process. The impossibility of measuring some parameters directly in some circumstances does not guarantee the kind of insight claimed in the literature. This is a characteristic of most models (van Brakel and Heertjes, 1974). The higher the number of such parameters, the worse the case.

Also, it is highly desirable to represent reality to the best of the experimental knowledge of the physical parameters available or to be measured. While the model should be realistic, it should be realizable for practical application and use. Besides it should be reliable to prevent mistakes at further stages of equipment design, developing drying schemes, and choosing optimum drying conditions (Sokhansanj, 1987). The quality features of the product should not be put in jeopardy.

A reliable description of the drying behavior of a product depends greatly on the accuracy in modeling the internal and external transports of energy and moisture. Drying of fermented cacao is fundamentally a process of simultaneous energy and mass transfer under transient conditions, as it is for many agricultural and food products. Therefore, a simulation model based on the principles of energy and mass conservation was derived. A distributive type of model was preferred because the transfers within the beans could be portrayed as a function of location and time (Jayas et al., 1991).

The model consists of a set of three nonlinear partial differential equations, representing general energy and mass balances for the product. Transport of water and acetic acid was included in the mass balances. The constitutive equations required for coping with the internal transfer mechanisms, the initial and boundary conditions for external transfer and completeness of the whole model were also derived. General assumptions underlying the process of development of the model are presented and discussed.

Drying of cacao involves supply of energy, usually by a convective medium, and driving off moisture. Moisture here may be considered as composed of water and the acetic acid produced during fermentation. Therefore, a simulation model to be used in this case has to cope with more than one mass transfer component. The model has to be, however, based on some assumptions required by the nature of the product. Fermentation induces some physical changes inside the beans. Cotyledons of fresh seeds are compact and smooth approximating a continuous structure. Fermentation causes their separation and reveal the actual physical appearance of the interior, that is, a pair of convoluted or

furrowed cotyledons (Cook, 1972, Wood 1975; Lehrian and Patterson, 1983). Figure 4.1 is a schematic drawing of beans cut open before and after fermentation.

Fermented beans exhibit some small and irregular canals that run and bifurcate in several directions, noticeably lengthwise, characterizing a highly complex internal geometry. Loss of compactness makes a realistic mathematical treatment of the problem virtually inconceivable. Consequently, there is need for working with effective parameters for mass and heat diffusion.

Constitutive Equations

Drying of agricultural products is a multicomponent transport process. The description of the flows involved in the process and their interactions may be based on the flux relations as derived in Appendix A. The theoretical concepts of irreversible thermodynamics were applied by Fortes and Okos (1981a,b) to develop a mathematical model capable of accounting for the major mechanism of moisture transfer in the drying of corn kernels.

For a product where the transport of heat and two mass compounds (water and acetic acid) take place, the following set of linear combinations may apply

$$\begin{aligned} \mathbf{J}_q &= L_{11}\nabla T + L_{12}\nabla \mu_w + L_{13}\nabla \mu_a \\ \mathbf{J}_w &= L_{21}\nabla T + L_{22}\nabla \mu_w + L_{23}\nabla \mu_a \\ \mathbf{J}_a &= L_{31}\nabla T + L_{32}\nabla \mu_w + L_{33}\nabla \mu_a \end{aligned} \qquad (4.1)$$

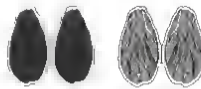


Figure 4 1. Sections of cacao beans (not to scale)
1 unfermented showing compact cotyledons (left)
2 fermented showing open cotyledons (right)

The fluxes of heat, water and acetic acid are functions of the straight and cross driving forces that is, the gradients of temperature water and the extra compound chemical potentials In other words the flux of energy is not only a function of the temperature gradient, but also of mass distribution Likewise, mass transports depend on the differences of chemical potentials and on thermal diffusion

Equations 4 1 form a set of constitutive equations. They describe the response behavior of a particular product in the course of a change process induced by one or more

driving potentials. Therefore, they allow for an understanding of the phenomena involved in such a process

Unfortunately, it is difficult to measure gradients of chemical potentials experimentally (Hines and Maddox, 1985) The equations mentioned above may be rewritten by expressing the driving forces in terms of gradients of temperature and concentrations of the chemical compounds involved in the process (Equation 4 2). Here the postulates of thermodynamics of irreversible processes do not apply. The matrix of coefficients K is not symmetric. Its elements are not constant and may take positive or negative signs Actually they are function of temperature and concentrations This approach is referred to in the mass transfer literature as the generalized **Fick's law** (Taylor and Krishna, 1993), combined with the Fourier law of heat conduction

$$\begin{aligned} \mathbf{J}_q &= -K_{qq}\nabla T - K_{qw}\nabla C_w - K_{qa}\nabla C_a \\ \mathbf{J}_w &= -K_{wq}\nabla T - K_{ww}\nabla C_w - K_{wa}\nabla C_a \\ \mathbf{J}_a &= -K_{aq}\nabla T - K_{aw}\nabla C_w - K_{aa}\nabla C_a \end{aligned} \tag{4.2}$$

In practice, the crosswise interference or influences are negligible and very often disregarded (Keey, 1972). Equations (4 2) may be simplified by assuming that the interference of acetic acid concentration on the other rates was negligible or had an effect at all This assumption may be founded on the fact that acetic acid is present at low concentrations In comparison with that of water it is smaller by a factor of nearly 100 for wet cacao

The equations were further modified and uncoupled by allowing for the dependence of the mass and thermal diffusivities on the concentration of water and

temperature. It was assumed that the diffusivity of acetic acid did not depend on its own concentration. Therefore, a set of equations analogous to those of Fourier for heat conduction and Fick for mass transfer was obtained as given below

$$\begin{aligned} \mathbf{J}_q &= -k\,\nabla T(\mathbf{x},t) \\ \mathbf{J}_w &= -D_w \nabla C_w(\mathbf{x},t) \\ \mathbf{J}_a &= -D_a \nabla C_a(\mathbf{x},t) \end{aligned} \tag{4.3}$$

Mass and Energy Balance Equations

Mass and energy balance equations were derived from the fundamental principles of conservation and they form the core of the mathematical model. The approach used here for formulating the general mathematical model is similar to that found in the literature on transport phenomena for homogeneous and heterogeneous flows (Aris, 1962, Standart, 1964, Slattery, 1967, 1981). It is usually called the macroscopic or integral formulation. It is preferred because it is more general compared to the differential procedure, since it applies to volumes of arbitrary shape and size. It consists of applying the basic conservation laws in integral form to a control volume to obtain the local intensive forms. Jump balances apply to variables that suffer discontinuities at phase change interfaces. A summary of the theoretical foundations and the derivation of the generalized equations are presented in Appendix B.

Mass Balance for the Dry Solids

Dry matter occupies the whole bean volume that shrinks during dehydration. If the assumption that the inside of cacao beans forms a continuous medium can be accepted, then no abrupt or sharp transition occurs with this component, even at the phase interface. Also no dry solid crosses the external surface, which moves due to shrinkage. There is no source or sink of dry matter in the medium, hence, the principle of conservation of mass assures that the total amount of utterly dry solids in the whole volume remains constant. The concentration of this component changes due to shrinkage, though. Since this constituent is conserved, the equation for conservation of mass derived in Appendix B can be used for the present purpose with slight modifications to obtain the following equation

$$\frac{\partial \rho_s}{\partial t} = -\nabla . \mathbf{J}, \qquad (4.4)$$

Inside the bean there is a flux of dry matter given by the velocity of shrinkage and transport of dry material occurs in the opposite direction of the transfer of moisture (Vagenas et al., 1990).

Balance Equation for Moisture

Moisture coexists in the wet product in both forms: liquid and vapor. A first assumption to make here is that there is a sharp and well delineated evaporating front within the beans. The liquid phase is confined by this surface interface. This phase

interface recedes at an arbitrary speed as drying proceeds The speed of displacement is equal to the component of the velocity vector with respect to the unit vector normal to the interface.

The bean shell is considered as part of the volume and, therefore, presents no extra resistance to mass transfer Thus is justifiable because it is relatively thin in comparison with the overall dimensions

Moisture is a component that is conserved in each phase (either liquid or vapor) but phase change from liquid to vapor occurs at the phase interface. At this surface instantaneous conditions of equilibrium are assumed to prevail Therefore, this situation is analogous to transport phenomena for more than one species The generalized balance equations for species and the jump conditions of flux at the singular interface are also derived in Appendix B Therefore, the following expressions may be used for moisture

1 Liquid phase

$$\frac{\partial \rho_l}{\partial t} + \nabla \cdot (\rho_l \mathbf{v}_l) = 0 \tag{4.5}$$

2 Vapor phase

$$\frac{\partial \rho_v}{\partial t} + \nabla \cdot (\rho_v \mathbf{v}_v) = 0 \tag{4.6}$$

3. Flux at the phase interface

$$\rho_l (\mathbf{v}_l - \mathbf{v}_b) \cdot \xi = \rho_v (\mathbf{v}_v - \mathbf{v}_b) \cdot \xi \tag{4.7}$$

The conversion of liquid into vapor, which is the actual flow phenomenon at the jump interface may be considered as sink of liquid and source of vapor in the corresponding

phases (Slattery, 1972). This is an analogy to heterogeneous chemical reactions. Thus the phase interface flux conditions may be added to the phase balance equations by expressing them in terms of rates of mass production and consumption, as appropriate

1 Liquid phase

$$\frac{\partial \rho_l}{\partial t} = -\nabla \cdot \mathbf{J}_l - I_l \tag{4.8}$$

2 Vapor phase

$$\frac{\partial \rho_v}{\partial t} = -\nabla \cdot \mathbf{J}_v + I_v \tag{4.9}$$

3 Both phases

$$\frac{\partial \rho_w}{\partial t} = -\nabla \cdot \mathbf{J}_w \tag{4.10}$$

Balance Equation for Acetic Acid

A reasoning similar to that used for moisture gives the following partial differential equation

$$\frac{\partial \rho_a}{\partial t} = -\nabla \cdot \mathbf{J}_a \tag{4.11}$$

Energy Balance Equation

Heat conduction and mass diffusion are analogous phenomena. Consequently, expressions corresponding to Equations 4.5 and 4.6 apply to the subregions, and 4.7 to the phase interface. This analogy leads to the following mathematical expression

$$\frac{\partial e}{\partial t} = -\nabla \cdot \mathbf{J}_q \tag{4.12}$$

This modeling approach may be further simplified by assuming that moisture evaporation takes place at the external surface. That is, the evaporation front and external surface coincide and move with matching displacement speed. For cacao this assumption is quite reasonable, at least during most of the drying process. Cacao has high initial moisture content and relatively low temperatures are used in drying to preserve its intrinsic characteristics, mainly those related to flavor. Such simplification leads to a model where the energy and mass balance equations become coupled by their boundary conditions. This may be accomplished by including terms that account for the latent heat of vaporization in the expressions for the boundary conditions. The contribution due to the evaporation of acetic acid may be neglected, since it is present in very small concentrations. Equation 4.4 needs not be solved formally. The bean volume may be allowed to change with moisture in the numerical procedure.

By expressing concentrations in terms of mass ratio based on the weight of the bone-dry material (dry basis) and substituting the energy content for an expression in terms of temperature, the following set of mass and energy balance equations are obtained:

$$\frac{\partial W}{\partial t} = \nabla.(D_w \nabla W)$$

$$\frac{\partial C_a}{\partial t} = \nabla.(D_a \nabla A) \qquad \textbf{(4.13)}$$

$$\rho c_p \frac{\partial T}{\partial t} = \nabla.(k\,\nabla T)$$

This is a set of nonlinear partial differential equations in the mass ratios of moisture (W), acetic acid (A) and temperature (T), since the thermal properties of the material and the diffusion coefficients vary with either temperature or moisture content or both. It is assumed that the transfer behavior inside the cacao beans is isotropic.

Initial and Boundary Conditions

These auxiliary conditions describe the physical situation at the start of a change process and on the boundary of the domain of the partial differential equations. They are required to guarantee the uniqueness of the model solution (Farlow, 1982). The initial distribution of the potential variables temperature moisture content and acetic acid mass ratio, may be assumed to be uniform and constant throughout the bean volume. The initial conditions for the model are given by the following expressions

1. Moisture

$$W(\mathbf{x},0) = W_o, \qquad \mathbf{x} \in V \tag{4.14}$$

2. Acetic acid

$$A(\mathbf{x},0) = A_o, \qquad \mathbf{x} \in V \tag{4.15}$$

3. Temperature

$$T(\mathbf{x},0) = T_o, \qquad \mathbf{x} \in V \tag{4.16}$$

The boundary conditions are given by the following relationships.

1 Moisture

$$-D_w\rho_s\frac{\partial W}{\partial \mathbf{n}} = h_w[Y(\mathbf{x},t) - Y(\infty,t)], \qquad \mathbf{x}\in S \tag{4.17}$$

This is a nonhomogeneous boundary condition of the third kind. The drying air humidity ratio depends on time.

2 Acetic acid

$$A(\mathbf{x},t) = 0, \qquad \mathbf{x}\in S \tag{4.18}$$

This is a homogeneous boundary condition of the first kind. Acetic acid concentration is assumed to be zero at the bean surface[1].

3 Temperature

$$-k\frac{\partial T}{\partial \mathbf{n}} = h_t[T(\mathbf{x},t) - T(\infty,0)] + h_w[Y(\mathbf{x},t) - Y(\infty,t)]H_{fg}, \qquad \mathbf{x}\in S \tag{4.19}$$

This boundary condition is more complex, since it involves latent heat of vaporization. The drying air temperature is constant. Other conditions are the same as before.

Introduction of the set of constitutive equations (4.3) into the corresponding balance equations (4.13) results in a set of partial differential equations that together with the auxiliary conditions make up the mathematical model to be solved.

[1]The use of this type of boundary condition for acetic acid is justifiable due to its higher volatility as compared to that of pure water. On evaporation, it diffuses quickly through the convective medium so as not to offer significant resistance at the air film that surrounds the product (Keey, 1972).

CHAPTER 5
MODEL SOLUTION

Equations 4 13 and their initial and boundary conditions 4 14 to 4 19 are the basis for the mathematical model developed to simulate the drying of cacao This is a set of nonlinear partial differential equations. They characterize propagation problems (Ames, 1977), with dissipative effects This type of equations is usually associated with diffusion processes (Anderson et al., 1984), where the fluctuations of the solution die or smooth out as the marching procedure progresses with time. These equations are not amenable to analytical solution, therefore a numerical procedure was used instead. Among the many numerical schemes available, the explicit finite difference technique was used

Finite Difference Approach

The basic idea underlying the formulation of finite difference methods is to represent the problem governing differential equations and their boundary conditions by discretized counterparts or approximate difference equations (Smith, 1978) As a consequence, approximations to the solution of the differential equations are searched for isolated and well defined points, rather than averywhere in the domain This leads to a set

of algebraic equations either linear or nonlinear, depending on the nature of the original differential equations.

Cacao beans have approximately an oval shape when fully wet, becoming flatter as moisture is lost. They were assumed to have the shape of finite slabs with average measured length, width and thickness. This simple geometry was adopted to reduce computational time because, if successful, this single bean model would be incorporated into a thick bed drying model.

The following mean ratios between length (l), width (w) and thickness (depth - d) apply to cacao beans

$$\begin{aligned} l/w &= 1.865 \quad \text{and} \quad w/d = 2.768 \\ d/l &= 0.361 \quad \text{and} \quad l/w = 0.674 \\ w/l &= 0.536 \quad \text{and} \quad l/d = 1.484 \end{aligned} \tag{5.1}$$

Typical mean values of these parameters are 2.439, 1.308 and 0.881 cm, respectively for length, width and thickness (Ghosh, 1976).

The assumed continuous domain was then replaced by a three dimensional discrete configuration or mesh with unequal node spacing in the x, y and z directions. Discretization of the domain was carried out for only one eighth of the slab volume because of the symmetry of the problem. This resulted in boundary conditions of no heat

flow for those nodes located on the surfaces of symmetry A view of the sectioned slab is shown in Figure 5 1

Each node in the network is associated with an elemental volume of regular shape bounded by plane surfaces, called node interfaces These interfaces are located between two consecutive grid points, perpendicular to the directing axis, at positions that depend on the sizes of the volumes associated with these nodes. The grid spacing was reduced toward the external surfaces of the slab to attain better accuracy in regions with steeper gradients

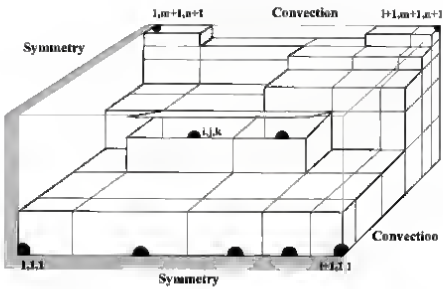


Figure 5.1. Partial view of the node network representation of the discretized solution domain

Discretization of a partial differential equation describing a physical process may be accomplished in different ways (Andersoo et al , 1984)

1 Taylor's series expansion and truncation

2. polynomial fitting

3 micro-integral method

4 control volume method

The last option was used here for the inherent advantages of this method of approximating the governing equations It allows for direct use of the fundamental conservation principles of physics, giving better insight into the phenomenon behind the problem to be solved. Numerical schemes derived from these principles are said to have the conservative property, that is, they maintain the conservation statement locally in the neighborhood of each mesh point, and throughout the domain, including the boundary nodes, in the process of assembling the single nodal difference equations. Such schemes represent the problem governing equation accurately and are said to be consistent (Andersoo et al , 1984) The Lax equivalence theorem guarantees that a consistent numerical scheme converges to the original partial differential equation if it is stable. Hence, the convergence problem reduces to that of finding the appropriate values of the increments in the independent variables to achieve stability (Ames, 1977).

Formulation of the difference equations was based on the three-dimensional stencil or computational molecule as depicted in Figure 5.2. In this fashion, the mass of each elemental volume of the spatial grid is considered as concentrated on the atoms of the molecule. The central sphere in the figure is highlighted for illustrating purposes only

It is connected by imaginary conducting rods to six surrounding nodes. This computational molecule represents a typical interior node with its associated elemental volume and interface areas. The axes x, y and z of the coordinate system are identified with the index letters i, j and k, respectively. Distances between two adjacent nodes are Δx, Δy and Δz in the corresponding directions

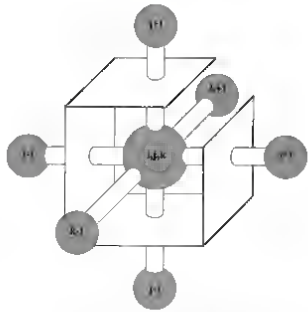


Figure 5.2 Node arrangement for a typical grid point in the interior of a three dimensional region.

Transient energy flows from the neighbors towards the central node of the computational molecule are balanced as in Equation 5 2 (Kreith and Black, 1980)

$$\begin{bmatrix} \textit{change in the internal energy} \\ \textit{of node } (i,j,k) \textit{ during } \Delta t \end{bmatrix} = \sum_{\substack{l=i\pm 1/2 \\ m=j\pm 1/2 \\ n=k\pm 1/2}} q_{l-i,j,k}$$

Using Fourier's law and an expression for the energy associated with the node (i,j,k) yield the following difference equation

$$\rho c_p \frac{(T^{t+\Delta t} - T^t)_{i,j,k}}{\Delta t} \Delta V =$$
$$k_{i-1/2} B_x \frac{(T_{i-1,j,k} - T_{i,j,k})^t}{\Delta x_i} + k_{i+1/2} B_x \frac{(T_{i+1,j,k} - T_{i,j,k})^t}{\Delta x_{i+1}} +$$
$$k_{j-1/2} B_y \frac{(T_{i,j-1,k} - T_{i,j,k})^t}{\Delta y_j} + k_{j+1/2} B_y \frac{(T_{i,j+1,k} - T_{i,j,k})^t}{\Delta y_{j+1}} +$$
$$k_{k-1/2} B_z \frac{(T_{i,j,k-1} - T_{i,j,k})^t}{\Delta z_k} + k_{k+1/2} B_z \frac{(T_{i,j,k+1} - T_{i,j,k})^t}{\Delta z_{k+1}} \qquad \textbf{(5.3)}$$

A method of treating the nonlinear thermal conductivity consists of averaging this property at two adjoining grid points (Finlayson, 1980) Therefore, the thermal conductivities, for example, $(k_{i-1/2})$ and $(k_{j+1/2})$ are evaluated as the average of the values of two connecting nodes, that is, the nodes $(i-1\ i)$ and $(i\ i+1)$, respectively

The terms on the right hand side of Equation 5 3 change if the nodes are located on the surfaces of symmetry and external faces of the slab There is no heat flow across the planes of symmetry and those nodes on the external surfaces exchange energy with the drying medium through convection and vaporization of moisture Nodes on the planes

of symmetry and on the external surfaces have characteristic dimensions that are different from those of the interior nodes. A subroutine was developed to calculate internodal distances, surface areas and volumes for the various types of nodes in the domain. Derivation of the various node equations is a repetitive task. Therefore, finite difference equations are presented for a few surface nodes, as examples.

Node $(1\ 1\ 1)$, the center node, has three surfaces of symmetry, which are equivalent to insulating surfaces, and three conducting rods. Therefore, this node is surrounded by three nodes with which it exchanges energy. Equation 5.3 can be modified as follows:

$$\rho c_p \frac{(T^{t+\Delta t} - T^t)_{i,j,k}}{\Delta t} \Delta V =$$

$$0 + k_{i+1/2} B_x \frac{(T_{i+1,j,k} - T_{i,j,k})^t}{\Delta x_{i+1}} +$$

$$0 + k_{j+1/2} B_y \frac{(T_{i,j+1,k} - T_{i,j,k})^t}{\Delta y_{j+1}} +$$

$$0 + k_{k+1/2} B_z \frac{(T_{i,j,k+1} - T_{i,j,k})^t}{\Delta z_{k+1}} \qquad (5.4)$$

A node located on the external surfaces, such as node $(l\ m\ n)$, exchanges heat by convection and through phase change with the medium. The corresponding difference equation is of the form

$$\rho c_p \frac{(T^{t+\Delta t} - T^t)_{i,j,k}}{\Delta t} \Delta V =$$

$$k_{i-1/2} B_x \frac{(T_{i-1,j,k} - T_{i,j,k})^t}{\Delta x_{i-1}} + h_c B_x (T_\infty - T_{i,j,k})^t +$$

$$k_{j-1/2} B_y \frac{(T_{i,j-1,k} - T_{i,j,k})^t}{\Delta y_{j-1}} + h_c B_y (T_\infty - T_{i,j,k})^t +$$

$$k_{k-1/2} B \frac{(T_{i,j,k-1} - T_{i,j,k})^t}{\Delta z_{k-1}} + h_c B_z (T_\infty - T_{i,j,k})^t - H'_{fk} \qquad (5.5)$$

where H_{fk} is the total heat loss owing to the amount of moisture vaporization associated with this particular node, and T_∞ is the temperature of drying air

The left-hand side of these equations refer to the time rate of accumulation of internal energy in the volume associated with the specific element. Since the specific heat capacity varies with temperature and moisture the numerical solution requires iteration to improve accuracy and, thus, to deal with the nonlinear nature of the differential equation For most situations two to three iterations are sufficient to attain the accuracy desired (Anderson et al 1984) Another approach is to calculate the properties for the current time level ($t+\Delta t$) at the temperature and moisture at the last time level (t) plus half the change in temperature and moisture during the last time step

The difference equations for moisture transfer are quite the same, except for the boundary nodes and transient term. By expressing the product moisture content as mass

ratio with respect to the mass of dry solids and using Fick's law instead of Fourier's, the following expression can be written

$$\frac{(W^{t+\Delta t}-W^{t})_{i,j,k}}{\Delta t}\Delta V =$$
$$D_{w_{eff}}B_x\frac{(W_{i+1,j,k}-W_{i,j,k})^t}{\Delta x_i}+D_{w_{eff}}B_x\frac{(W_{i+1,j,k}-W_{i,j,k})^t}{\Delta x_{i+1}}+$$
$$D_{w_{eff}}B_y\frac{(W_{i,j-1,k}-W_{i,j,k})^t}{\Delta y_j}+D_{w_{eff}}B_y\frac{(W_{i,j+1,k}-W_{i,j,k})^t}{\Delta y_{j+1}}+$$
$$D_{w_{eff}}B_z\frac{(W_{i,j,k-1}-W_{i,j,k})^t}{\Delta x_k}+D_{w_{eff}}B_z\frac{(W_{i,j,k+1}-W_{i,j,k})^t}{\Delta z_{k+1}} \qquad (5.6)$$

The numerical solution of this equation requires no iteration. The procedure to approximate the values of mass diffusivity between two adjacent nodal points is the same as that used for thermal conductivity.

Nodes on the surfaces of symmetry are treated exactly in the same way as in the preceding case. Those on the external surfaces exchange moisture through convection with the drying air. This process is analogous to heat transfer by convection without phase change. Therefore, the difference equation (5.7) can be applied. Conditions of equilibrium on the external boundaries are assumed to exist. This implies that the vapor pressure on the external surface equals that of the air in close contact with the product. In the expression below this situation is given in terms of humidity ratio (Y_s) of the air in equilibrium with the moisture content of the surface volume elements. The driving force is the difference between this humidity ratio and that of the drying air. Conditions of

equilibrium can be obtained from curves of moisture isotherms determined for the product. The density of the bone dry material (ρ_b) is constant

$$\frac{(W^{t+\Delta t} - W^{t})_{i,j,k}}{\Delta t}\Delta V =$$
$$D_{w,n} B_x \frac{(W_{i-1,j,k} - W_{i,j,k})^{t}}{\Delta x_{i-1}} + \frac{h_w}{\rho_b} B_x (Y_m - Y_s)^{t} +$$
$$D_{w,n} B_y \frac{(W_{i,j+1,k} - W_{i,j,k})^{t}}{\Delta y_{j}} + \frac{h_w}{\rho_b} B_y (Y_m - Y_s)^{t} +$$
$$D_{w,n} B_z \frac{(W_{i,j,k-1} - W_{i,j,k})^{t}}{\Delta z_{k-1}} + \frac{h_w}{\rho_b} B_z (Y_m - Y_s)^{t} \qquad (57)$$

Equations for acetic acid are developed with the same approach used for moisture. The boundary conditions on the external surfaces are simpler, however. Zero concentration was imposed at the elements on these surfaces. For the external boundary nodes

$$\frac{(A^{t+\Delta t} - A^{t})_{i,j,k}}{\Delta t}\Delta V = D_{a} B_x \frac{(A_{i+1,j,k} - A_{i,j,k})}{\Delta x_{i}} +$$
$$D_{a,n} B_y \frac{(A_{i,j+1,k} - A_{i,j,k})}{\Delta y_{j-1}} + D_{w,n} B_z \frac{(A_{i,j,k-1} - A_{i,j,k})}{\Delta z_{k-1}} \qquad (58)$$

For the other node types the finite difference equations match exactly the corresponding equations derived for moisture transfer.

Stability Criterion

The temperature difference equations for interior nodes, as represented by Equation 5.3, can be rearrange to yield expressions explicit in terms of temperature T at time $t+\Delta t$.

$$
\begin{aligned}
&T_{i,j,k}^{t+\Delta t} = \\
&\frac{k_{i-1/2}}{\rho c_p}\Delta t\frac{B_x}{\Delta x_i \Delta V}T_{i-1,j,k}^{t} + \frac{k_{i+1/2}}{\rho c_p}\Delta t\frac{B_x}{\Delta x_{i+1}\Delta V}T_{i+1,j,k}^{t} + \\
&\frac{k_{j-1/2}}{\rho c_p}\Delta t\frac{B_y}{\Delta y_j \Delta V}T_{i,j-1,k}^{t} + \frac{k_{j+1/2}}{\rho c_p}\Delta t\frac{B_y}{\Delta y_{j+1}\Delta V}T_{i,j+1,k}^{t} + \\
&\frac{k_{k-1/2}}{\rho c_p}\Delta t\frac{B}{\Delta z_k \Delta V}T_{i,j,k-1}^{t} + \frac{k_{k+1/2}}{\rho c_p}\Delta t\frac{B}{\Delta z_{k+1}\Delta V}T_{i,j,k+1}^{t} + \\
&\left\{1-\Delta t\left[\left(\frac{k_{i-1/2}}{\rho c_p}\frac{B_x}{\Delta x_i \Delta V}+\frac{k_{i+1/2}}{\rho c_p}\frac{B_x}{\Delta x_{i+1}\Delta V}\right)+\right.\right. \\
&\left(\frac{k_{j-1/2}}{\rho c_p}\frac{B_y}{\Delta y_j \Delta V}+\frac{k_{j+1/2}}{\rho c_p}\frac{B_y}{\Delta y_{j+1}\Delta V}\right)+ \\
&\left.\left.\left(\frac{k_{k-1/2}}{\rho c_p}\frac{B}{\Delta z_k \Delta V}+\frac{k_{k+1/2}}{\rho c_p}\frac{B}{\Delta z_{k+1}\Delta V}\right)\right]\right\}T_{i,j,k}^{t}
\end{aligned}
\qquad (5.9)
$$

According the maximum principle, the coefficients for temperature on the right-hand side of Equation 5.9 should be nonnegative and sum to one (Ames, 1977).

This fact allows for the calculation of the stability criterion or the value of the time increment to attain stability for the energy equation. Specifically, Δt has to be such that the coefficient associated with $T_{i,j,k}$ at time t in Equation 5.9 is equal or greater than zero. The same criterion has to be applied to all finite difference equations involving Δt.

Computer Algorithm

A computer program was written in FORTRAN to implement the numerical solution of the model. A listing of the program is given in Appendix E. The flowchart of Figure 5.3 shows the major subroutines used by the main program to carry out the numerical procedure. The main program, module CACAO DRYING, consists of three nested loops for the three independent space variables inside a fourth loop for time. In addition, it is used to input process data and to output results from the computations.

Subroutine GRID is used to calculate the geometric parameters for the spatial mesh used in the numerical solution of the model. It is called inside the time loop to assemble the initial space discretization and then to update the mesh characteristics to reflect physical changes due to moisture content. The subroutine GRID generates nodes in the three directions that are not equally spaced, so as to have nodes with smaller volumes near the external boundaries (Figure 5.1).

Modules TEMPERATURE, MOISTURE and ACETIC ACID are called inside the four loops to compute temperature, moisture content and acetic acid concentration at each grid point and time step. The marching procedure starts at the most internal mesh

point, node ($1\ 1\ 1$) and proceeds outwardly until the most external point is reached, node (l,m,n). The computations for each time increment are done using data from the previous time level

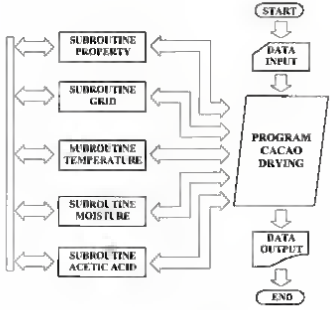


Figure 5.3. Simplified flow chart of the computer algorithm used to implement the drying model numerical solution

The block PROPERTY, in the diagram, comprises a set of modules to compute product properties and drying air physical and psychrometric parameters. It also includes other auxiliary modules to compute average versus time profiles for the dependent variables. In addition, four subroutines of the Numerical Recipes Software package (Press et al , 1992) were also incorporated into the program to be used in the procedure

for estimating mass diffusivity They were used to fit cubic splines to the drying data, compute slopes of drying curves perform numerical interpolation and to search ordered tables of data

The main module and the subroutines GRID TEMPERATURE, MOISTURE, ACETIC ACID and some modules of the PROPERTY block share data stored in common blocks of memory (Figure 5.3)

The program was tested and used to appraise the response behavior of the model solution to changes in some input parameters namely domain dimension, grid refinement and time increment, shrinkage time step, drying air relative humidity and velocity A modified version of the original program was employed to determine mass diffusivity from the drying data. Then CACAO DRYING was used to simulate the drying process of cacao beans to validate the proposed model

CHAPTER 6
EXPERIMENTAL PROCEDURES

Due to the lack of availability of cacao in Florida and the susceptibility to quick deterioration of the fermented beans , the research experimental work was carried out at the Brazilian Cocoa Research Center in Itabuna, Bahia State, Brazil

Sample Preparation

The product used in the experimental tests was cacao extracted from ripe and partially ripe pods kept in the field for two to three days after removal from the trees. The fresh seeds were taken to the fermentary and fermented regularly for six days in 1 m^3 batches, following standard procedures and recommendations for turning and aeration of the product during the process. After completion of fermentation, samples of approximately 12.5 kg were taken weekly from a single fermentation box and stored for no more than one week in a home freezer. This amount of cacao was sufficient to carry out the set of four drying tests planned for five to six working days. Prior to cold storage, the samples from the fermenter were divided into four 2.5 kg samples and placed into plastic bags. The test samples were taken from the freezer the day before and left at ambient temperature (between 25 and 30 °C) overnight to defrost and equilibrate to room

temperature This process required from 16 to 20 hours. Each set of tests consisted of four drying temperatures and one air velocity

Drying Tests

Drying tests of fully exposed cacao beans were carried out to obtain moisture and acetic acid loss curves to determine the effective diffusivities for these compounds and to validate the mathematical model These tests were done in a laboratory drier depicted in the schematic diagram of Figure 6 1

The test drier consisted of a centrifugal blower driven by a 0 375 kW and 2850 RPM motor that delivered ambient air to a bank of four electric resistance heaters with a combined rating of 7 5 kW A control panel was used for controlling the system operation. The electric current to one of the resistors was controlled by a Foster Cambridge Clearspan (model P130L) controller The drying air temperature could be maintained to within ± 0 6 °C of the set value The test sample was held on the screen tray (0 3 m in diameter), seated on a conical plenum chamber The air velocity was measured with a Lambrecht KG vane anemometer Temperature of the drying air and ambient air dry bulb and wet bulb temperatures were monitored by means of type K thermocouples (chromel alumel 24 AWG) connected to a 12-point Foster Cambridge temperature recorder

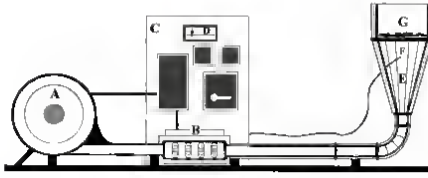


Figure 6.1. Schematic representation of the laboratory drier showing centrifugal fan (A) heater bank (B) control panel (C) with temperature controller (D) plenum (E), temperature sensor (F) and drying tray (G)

The temperature recorder was calibrated against an Omega Engineering precision calibrator, model CL 6503 (resolution 0.1 °C, accuracy ± 0.5 °C) at the beginning of each test run Then its readings were checked periodically with a Comark electronic thermometer with resolution and accuracy comparable to those of the calibrator

Air temperatures of 40, 50, 60 ,70 and 80 °C were used in the drying tests. The last value was used in the tests with the highest air velocities only Temperatures above this range are not recommended for cacao since higher temperatures interfere with enzymatic reactions that occur within the product during this process The lower limit of this range

is close to the temperature values experienced by the product dried in the sun under the prevailing conditions in Bahia. Sun drying is also often used as a control for experiments designed to investigate effects of preconditioning variables on the quality of cacao and chocolate.

The values of airflow rate used to determine the effective mass diffusivities were chosen based on data available in the literature for products of similar size (Masi and Riva, 1988). These data were the starting point for a set of preliminary tests to find the lowest limit of air velocity that did not interfere with the kinetics of cacao drying. These tests showed that the process kinetics were not affected by velocities above 1.8 to 2.0 m/s.

The four air velocities used in the tests were about. 0.1, 0.5, 1.0 and 2.5 m/s. The highest value was used to determine the effective mass diffusivities. The three lower values are within the airflow range used for cacao. A summary of the test conditions are given in Table 6.1.

The drying curves were obtained by periodic weighing of a smaller sample, approximately 0.1 kg, kept in plastic tray placed in the drying tray of Figure 6.1. Weighing was done manually on a Mettler balance (model PL320) with capacity for up to 320 g, resolution of 0.01 g.

The concentrations of the most important acids found in fermented cacao beans were monitored by taking samples of about 10 g from the drying tray at variable time intervals. These samples were processed for extraction and quantification of citric, lactic and acetic acids.

Table 6.1 Conditions of the drying air used in the experimental tests

Velocity (m/s)	Temperature (°C)
0.1	40
	50
	60
	70
0.5	40
	50
	60
	70
1.0	40
	50
	60
	70
2.5	40
	50
	60
	70

Sample Acidity and Moisture Content Determinations

Acid concentrations were measured using high pressure liquid chromatography (HPLC) The system used (Gilson France S A.) consisted of

1. Gilson pump (model 302)
2. Gilson pressure controller (model 802)
3. Brukker IR detector (model 9E 00)
4. CG integrator/processor (model 300)
5. BIO-RAD fermentation monitoring column (150x7 8mm) for sugars, organic acids and alcohols

The following procedures were used for citric, lactic and acetic acids

1. Extraction
   - i. grinding of approximately 6 g of beans in home blender
   - ii. mixing with 50 g of distilled water
   - iii. homogenization for less than 2 minutes
   - iv. centrifugation for about 5 minutes at 5000 RPM
   - v. filtration in filtrate membrane with pore diameter of 0 25 μm
2. Acid quantifications
   - i. injection of 20 μl aliquot
   - ii. solvent used H_2SO_4 0 005 N

iii. flux of 0.5 ml/min

iv. temperature of approximately 25 °C (ambient)

v. duration of approximately 15 minutes

vi. number of injections per sample: 2 or 3 depending on the repeatability of two consecutive outputs

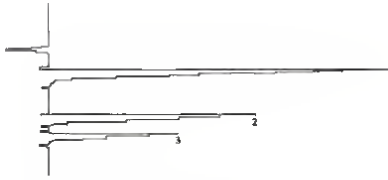
The instrument was calibrated at the beginning of each use by external standardization and checked daily. A standard mixture containing 0.4% of acetic, lactic and citric acid was used. Figure 6.2 shows an example of the chromatogram obtained in the process of calibration of the equipment.

Moisture contents of wet and dry samples were determined by drying the beans in a ventilated oven at a temperature of 105 ± 2 °C for 24 hours.

Product Physical Properties

Solution of the drying model requires the availability of data for some parameters of the product which usually depend on its temperature and moisture content. The following properties were needed:

1. Geometrical characteristics: bean size (length, width and thickness), area and volume.
2. Thermal properties: specific heat capacity, thermal conductivity, latent heat of moisture vaporization and convective heat transfer coefficient.
3. Mass transfer properties: mass diffusivity, equilibrium moisture content and convective mass transfer coefficient.



CROMATOPACK C-R3A

PKNO	TIME	AREA	CONC	NAME
1	5.448	775218	0.3965	CITRIC ACID
2	8.458	624478	0.3895	LACTIC ACID
3	10.303	469923	0.3876	ACETIC ACID

Figure 6.2. Typical calibration chromatogram for the high pressure liquid chromatographer

The length (*l*), width (*w*) and thickness (*d*) of the beans, as illustrated in Figure 6.3, were measured experimentally using a caliper. Drying tests were carried out to measure changes in size with moisture contents. Beans randomly marked , no less than ten, from wet samples of approximately 1 kg were measured and weighed periodically during the drying process. Actual bean volume was measured with a pneumatic picnometer constructed specially for cacao beans (Prado et al. 1981). For computation purposes, surface areas and volumes were calculated from the length, width and thickness, assuming a finite slab shape. The relationships between these parameters and

moisture content were determined by means of polynomial regression, following the procedure described by Littel et al. (1991).

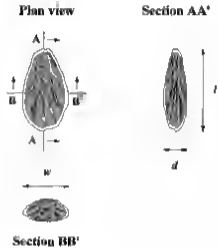


Figure 6.3 Definition of cacao bean dimensions (not to scale) length (l), width (w) and thickness(d)

The effect of temperature was not assessed, since it is normally not noticeable. Furthermore the ranges of drying air temperatures used for cacao are not very high, a maximum of about 40 °C above ambient.

The following empirical expressions were obtained from the literature for the specific heat and thermal conductivity of fermented cacao beans (Sasseron, 1984)

$$c_p = 3090 + 1820W - 1580W^2 \qquad (6.1)$$

$$k = 0.18 + 0.266W - 7.81 \times 10^{-4} T \qquad (6.2)$$

A mathematical expression for the latent heat of vaporization was derived from moisture sorption isotherm equation, available for cacao, following the procedure used by Balaban et al. (1987). This methodology is based on the Clausius-Clapeyron equation and it takes into consideration the thermodynamics of the sorption process that imposes some restrictions on the range of applicability of the sorption isotherm equation selected to fit sorption data for a product. The heat involved in a pure sorption process should decrease with the moisture content of the material or its temperature.

Sorption data available in the literature were almost exclusively determined for applications to storage problems. They were measured through moisture uptake rather than desorption methods. Furthermore, they are restricted to very narrow temperature ranges around the ambient temperature.

The expression of Equation 6.3 represents the Day and Nelson's modified Henderson equation for fermented cacao beans as determined by Duque (1974). It covers a broader temperature range and was used in this work.

$$a_w = \exp\left(6.414 \times 10^{-34} T^{10.43} W^{4.688 \times 10^4 T^{-17.4}}\right) \qquad (6.3)$$

Convective heat transfer coefficients were calculated from the general expression determined by Pasternak and Gauvin (1960) for single particles of several shapes and orientations with respect to the fluid flow (Equation 6.4). The characteristic dimension used to compute the Reynolds number (Re) is defined as the ratio of the total surface area

to the maximum length of the perimeter of the body projected area perpendicular to the flow Equation 6 4 is valid for Reynolds numbers in the range of 500 to 5000

$$j_c = \frac{h_c}{\rho_{ar} v_\infty c_{p_{ar}}} \mathrm{Pr}^{2/3} = 0.692\,\mathrm{Re}^{-0.486} \qquad (6\,4)$$

The empirical analogy of equality of the Chilton-Colburn j-factors for both heat and mass transfer by convection (Bird et al , 1960) leads to the following expression for the convective mass transfer coefficient

$$j_w = \frac{h_w}{v_\infty} \mathrm{Sc}^{2/3} = 0.692\,\mathrm{Re}^{-0.486} \qquad (6\,5)$$

Equation 6 5 is valid for gases and liquids with Sc and Pr numbers in the range of 0 6 to 2500 (Skelland, 1985).

Mass Diffusivity

Mass diffusivity is an indispensable transfer property in mathematical modeling and simulation of drying processes. This parameter depends on the product temperature and moisture content. No direct method can adequately cope with products of irregular shape In this case, analysis of drying data is a technique that can be used to determine effective values for mass diffusivity

The analytical solution of the partial differential equation that governs diffusion in a brick-shaped solid may be given by the product solution or Newman's rule (Fahlen, 1983). The end result comes from the product of the individual infinite slab

solutions in the three directions of a rectangular coordinate system. Hence, the distribution of a general dependent variable in space and time can be described as

$$M(x,y,z,t) = M(x,t)M(y,t)M(z,t) \tag{6.6}$$

The individual solutions, may be given in terms of infinite series expansion (Mikhailov and Ozisik 1984)

Average dimensionless concentration can be obtained by integrating the solution of Equation 6.6. For a rectangular parallelepiped of dimensions 2*l*, 2*w*, 2*c*, constant initial distribution, prescribed boundary conditions and large enough times the series solution simplifies to (Fahien, 1983)

$$M(t) = 64\frac{8}{\pi^6}\exp\left[\frac{D\pi^2 t}{4(l^2+w^2+d^2)}\right] \tag{6.7}$$

This expression was used to estimate effective mass diffusivities from the slopes of the plots of the experimental values of $\ln[M(t)]$ versus time. The slopes needed were evaluated by means of cubic spline approximation, numerical interpolation and differentiation (Press et al., 1992). With this procedure, it is possible to relate mass diffusivity to product moisture content and temperature. Similar relationships have been used for grains and food products (Tong and Lund, 1990)

$$D = \alpha\exp\left(\beta W + \gamma W^2 + \delta W^3 + \frac{\lambda}{T}\right) \tag{6.8}$$

where α, β, γ, δ and λ are regression parameters

This mathematical model has inherent statistical properties that motivated its choice It is not too complex as compared to others that are available and the regression parameters inside the brackets have similar close-to-linear estimation behavior (Ratkowsky, 1990) This allowed the use of linear regression with linearization by logarithm transformation without incurring significant errors. The same procedure may be applied to find a similar mathematical relationship for the diffusivity of acetic acid

There is a small limitation to the above procedure The assumption underlying Equation 6 7, that is, its validity only for large values of time, makes it not suitable for determination of mass diffusivity at the beginning of the drying process If the above procedure were applied during the initial stage of drying the resulting mass diffusivity would be lower than the actual value because Equation 6 7 does not reflect the time lag phenomenon at the beginning of the drying process. These values should not be used in the regression analysis to determine the parameters of Equation 6 8

CHAPTER 7
RESULTS AND DISCUSSION

This chapter includes presentation and discussion of the results obtained during testing of the computer program developed to simulate the drying process of fermented cacao as well as its output behavior as function of variation in some model parameters and drying conditions. The experimental results presented and discussed are data obtained for physical properties, moisture loss, mass diffusivity, outcomes from the model validation and product acidity. Acidity was expressed and assessed in terms of concentrations of the most important acids found in cacao beans, namely: citric, lactic and acetic acids.

Product Physical Properties

The physical properties of the product and the latent heat of moisture vaporization play an important role in the solution of the drying model equations. Therefore, they have to be analyzed with respect to the accuracy with which they were measured. The following sections presents the results of bean size measurements, their changes with respect to moisture content and the total heat of vaporization at different temperatures and moisture contents.

Geometric Characteristics and Bean Mass

Linear regression was used to analyze the data obtained for the properties associated with cacao bean size, namely: length, width, thickness, volume and mass. The following regression equations were determined (dimensions expressed in millimeters):

1 Length.

$$l = 23.058 + 1.178W - 1.306W^2 + 1.630W^3 \quad \textbf{(7.1)}$$

standard deviation estimate: 0.362
multiple correlation coefficient: 0.8201

2 Width.

$$w = 13.191 + 1.374W - 3.839W^2 + 5.070W^3 \quad \textbf{(7.2)}$$

standard deviation estimate: 0.100
multiple correlation coefficient: 0.9896

3 Thickness.

$$d = 6.724 + 0.835W + 4.317W^2 - 2.674W^3 \quad \textbf{(7.3)}$$

standard deviation estimate: 0.163
multiple correlation coefficient: 0.9805

4 Volume (mm^3)

$$V = 2072.672 + 222.161W + 1619.861W^2 - 481.345W^3 \quad \textbf{(7.4)}$$

standard deviation estimate: 89.708
multiple correlation coefficient: 0.9817

5 Bean mass (g)

$$m = 0.970 + 0.936W \quad \textbf{(7.5)}$$

standard deviation estimate: 0.002
multiple correlation coefficient: 0.9996

These regression equations are valid for moisture contents within the range of 0 07 to 1 30 (dry basis) The lower values of the mean square error and multiple correlation coefficient associated with Equation 7 1 reflect a greater degree of variability of the bean length in relation to the other dimensions This seems to be a characteristic of the material itself, rather than measurement errors.

The plots shown in Figure 7 1 are for average dimensionless values of these properties versus moisture content obtained in the experiments done for size measurements Nondimensionalization was carried out by expressing the parameters in terms of the ratios of their actual values to the corresponding initial values. Due to the internal structure of the bean, the change in the size of the bean during drying is not the same in all directions

Unfermented cacao seeds are flat and characterized by a compact and smooth interior Upon fermentation the convoluted cotyledons (Wood, 1975) tend to separate from each other as a consequence of the incipient germination and penetration of liquids resultant from the fermentation process Separation occurs sidewise and in the direction of the thickness, but not in the direction of the largest dimension (length) This phenomenon tends to make the beans to become plump as compared to the unfermented flat seeds, and to loosen the hull from the cotyledons after roasting During drying the reverse takes place, that is, the cotyledons tend to go back to their initial position, thus the existence of differentiated size reduction. The initial position state is not fully achieved Reduction of the bean thickness with moisture losses was remarkably larger than size reductions in the other directions. Thickness decreased by approximately 25% of its

initial value, as compared to nearly 12.5% and less than 5% for the bean width and length, respectively. Shrinkage caused by desorption of moisture itself was comparably smaller. Most of the volume reduction observed was due to partial restoration of position of the cotyledons inside the bean case, rather than contraction of the solid skeleton, owing to the hygroscopic properties of the material.

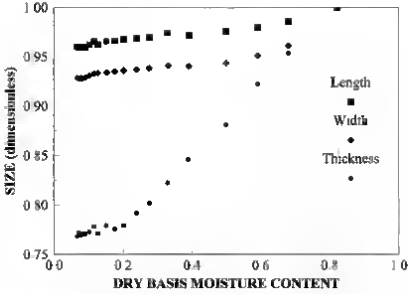


Figure 7.1. Relative size changes of fermented cacao beans with moisture content.

Relationships for Equilibrium Moisture Content and Latent Heat of Vaporization

The mathematical expression used to compute the latent heat of vaporization of bound moisture was derived from the relative humidity-equilibrium moisture content relationship by Duque (1974) as in Equation 6.3 of Chapter 6.

$$a_w = 1 - \exp\left[AT^B W^{(C+D)} \right] \tag{7.6}$$

where A = -6 414×10^{-5}
B = 10 43
C = 4 688×10^{4}
D = -1 714

Predictions of equilibrium moisture content from this relationship are plotted against values of water activity in Figure 7 2, for temperatures in the range of 20 to 70 °C Equilibrium moisture content of fermented cacao is somewhat lower than that of unfermented beans and other products when compared at the same conditions. The loss of compartmentalization of the internal structure of the seed during the fermentation process brings moisture and butter in close contact. Cacao butter, being a hydrophobic substance, repels water when both are put together This fact explain the relatively lower equilibrium moisture content and it is also the reason why fermented cacao has to be dried to a much lower moisture content, 7 to 8% (wet basis), before it can be stored and marketed The curves of Figure 7 2 show that most of the equilibrium moisture is within 0 to 0 125 for values of water activity less than 0 8

The total heat of moisture vaporization in the drying process comprises the heat of desorption (H_d) plus that required to evaporate water (H_v) in free state

$$H_{fg} = H_d + H_v \tag{7.7}$$

The first term in Equation 7 7, the desorption heat, depends on the product moisture content and temperature and should decrease with increasing moisture and temperature

The heat of vaporization of free water is a function of its temperature and may be computed by means of several expressions for saturation vapor pressure available Usually these relationships lead to equations for the latent heat of vaporization that satisfy the condition that this property should also decrease with increasing temperature The expression used in this study was the one determined by Wexler and Greenspan (1971) Its predictions of saturation vapor pressures and those from several other relationships available agree very well for temperature within the range of 0 to 100 °C (Wilhelm 1976) Although it is relatively more complex, it is sometimes recommended because it is founded on more recent data.

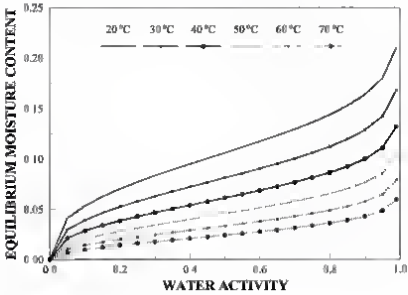


Figure 7.2 Calculated data of equilibrium moisture content for fermented cacao beans using Equation 7.6

By using the analytical procedure developed by Baliban et al (1987), the following expression was derived

$$H_R = R\left[\frac{-\exp\left[AT^B W^{(CT^D)}\right]}{1-\exp\left[AT^B W^{(CT^D)}\right]}\right]\left[AT^B W^{(CT^D)} T\right]\left[B+\ln(W)CDT^D\right]+H_v \qquad (7.8)$$

where A, B, C and D are the same as in Equation 7 7, and R is the ideal gas constant.

Computed results obtained from this equation are plotted against product moisture content and temperature, respectively, in Figures 7 3 and 7 4 These curves have negative slopes indicating that the latent heat of moisture vaporization decreases with increasing temperature and moisture content.

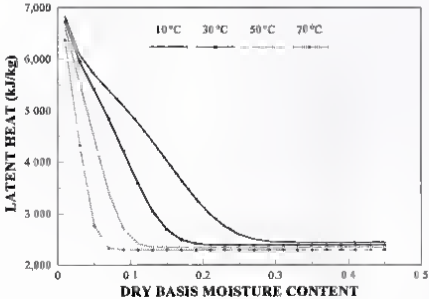


Figure 7.3 Total vaporization heat of bonded moisture in fermented cacao beans for different temperatures

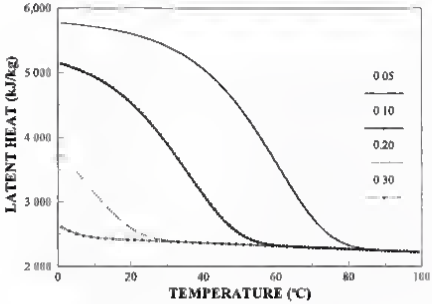


Figure 7.4 Total vaporization heat of bonded moisture in fermented cacao beans for the moisture content range of 0 05 to 0.30

It can be verified from these graphs that, for higher temperatures, the heat of desorption decreases with increasing moisture content and approaches that of pure water, under the same temperature, very quickly (Figure 7 3) Figure 7 4 shows that this property is significantly higher than that of water in the range of temperature studied, for lower moisture contents This indicates that the desorption heat of fermented cacao beans is important in drying simulations, since this product has to be dried to quite low moisture contents

Program Testing and Parameter Analysis

The computer program was used to test some parameters under restricted conditions. Parameters investigated were associated with the numerical technique used, that is the explicit finite difference method. Number of domain dimensions, node number, node spacing and the time step required to guarantee a stable and accurate solution comprised the set of parameters studied.

Initially, the dimension number was analyzed aiming at a reduction in the time required to run the computer program. These tests were carried out with the subroutine written to solve for the energy equation. Values of parameters and conditions used in these runs are given in Table 7.1. These values were taken from the literature, either for cacao or for other products with similar geometry and dried under conditions that are somewhat alike. The results obtained showed that the reduction of the number of dimensions could lead to quite different solution profiles. Therefore, the possibility of reducing the dimension number for the problem was discarded. Curves for change of the mean temperature with time are shown in Figure 7.5 for wet product. Since all flow controlling parameters were held constant throughout the simulations of the heating process, the different rates of temperature increases are due to differences in the total surface area of the slab. A finite brick shaped slab has greater external surface for heat exchange with the convective medium. The results from the numerical and analytical solutions compared very well, confirming the accuracy of the finite-difference solutions

Table 7.1. Values of parameters product and air temperatures used to generate the temperature profiles of Figure 7.1

Specific heat (kJ/kg °C)	3500
Thermal conductivity (W/m °C)	0.4
Convective heat transfer coefficient (W/m² °C)	50
Bean length (m)	$2.0\ 10^{-3}$
Bean width (m)	$1.0\ 10^{-3}$
Bean thickness (m)	$0.6\ 10^{-3}$
Product mass density (kg/m³)	1500
Product temperature (°C)	25
Air temperature (°C)	50

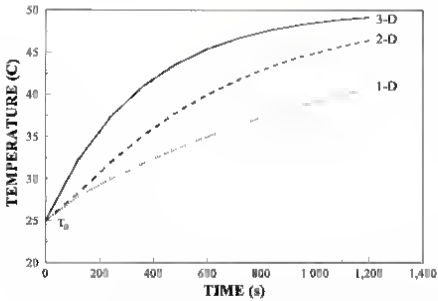


Figure 7.5. Average temperature profiles from computations for 1, 2 and 3 dimensional domains.

Trial runs to determine the stability conditions of the finite difference scheme were done with the subroutines developed to solve for the product moisture content and temperature. At first, the subroutines were tested separately and later they were coupled. These tests were conducted for constant moisture diffusivity coefficient and thermal properties. The values of moisture diffusivity and drying air temperature used were 6.9×10^{-9} m/s^2 and 70 °C, respectively. Both values are relatively high. This choice was made on purpose to have answers in short run times and to obtain safe time step values. For a given internodal space configuration, the higher the diffusivity the lower the time step required to achieve stability. A time step of 0.25 s was needed to obtain stability, when the cacao bean was represented by 12 nodal points in each of the three perpendicular directions.

Results of average moisture content computed for some node number combinations are shown in Figure 7.6 as a function of time. Node number combinations are expressed in terms of nodal point numbers, sequentially, in the length (l), width (w) and thickness (d) directions. Uniform spacing was used in these computational networks. The same curve pattern was obtained for the simulated temperature profiles, except that the product temperature increases during the drying process.

Networks with unequally spaced nodes were investigated in association with node number combinations. Finer mesh size was used near the slab external surfaces, where the dependent variables experience steeper gradients. In this way, results obtained with smaller numbers of nodes could be comparable to those from finer grids. The node number combination of 6x6x6 used with this type of network produced average moisture

profiles that agreed well with those for larger number of nodes in networks with equal internodal spaces A schematic representation of the node distribution used is depicted in Figure 7 7 It is shown for one direction only for the sake of simplicity

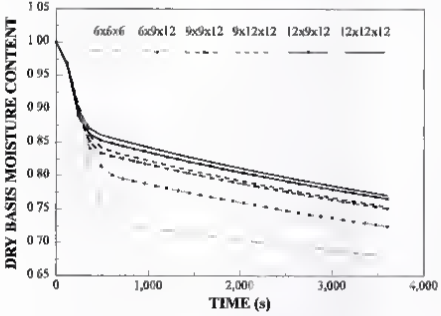


Figure 7.6. Comparison of average moisture profiles for different combinations of equally spaced node numbers

The element volume interfaces were positioned so as to generate 10, 15, 25 and 50-percent node types Centered nodal interfaces produced the 50-percent node type. Positioning of the interfaces closer to the most external nodes, at points 10, 15 and 25% from these nodes generated the corresponding type of mesh These percentages also correspond to the size of the volumes associated with the external nodes, relative to the

distance between them and their immediate internal neighbors Hence the terminology 10- 15, 25 and 50-percent external nodes

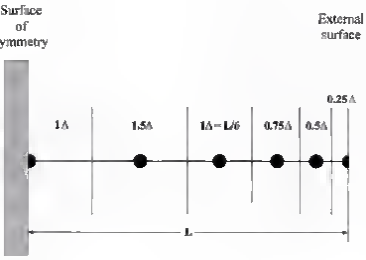


Figure 7.7. Node distribution along one direction axis for non-uniform spacial grid.

The average moisture and temperature profiles presented in Figure 7 8 are for different types of external nodes, as described above External nodes of the 50-percent type yielded poorer results when compared with nodes associated with smaller volumes, while 10-percent nodes eventually induced instability in the computations, as a consequence of shrinkage This type of node required a much shorter time step (0 1 s) to achieve stability Results from computations done for 15-percent and 25 percent nodes were comparable to those obtained for 10-percent nodes The maximum discrepancy

verified for moisture computed with the mesh used a 6x6x6 grid with 25-percent external nodes, and the grid with 12x12x12 equally spaced nodes was about 0 02 and average difference less than 0 014

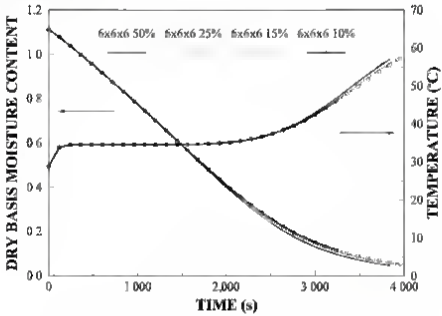


Figure 7 8. Comparison of average moisture and temperature profiles for different external node volume sizes

Effect of Shrinkage

Cacao beans undergo considerable weight loss and volume reduction in the course of the drying process as shown in Figure 7 9. The total volumetric change, when wet beans are dried to a moisture content of about 0 20 (dry basis) is approximately half of

their initial volume. Below this moisture content, volume change is negligible. Loss of weight to obtain dry cacao is about the same order of magnitude.

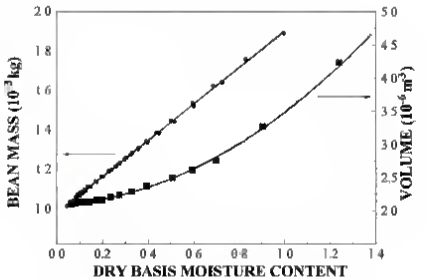


Figure 7.9. Change in cacao bean volume and mass with moisture content

To investigate the effect of this parameter on the predicted data, the bean volume was adjusted according to its dependence on moisture. Linear regression was used to fit cubic polynomials to the experimental data obtained for the bean geometric dimensions. Computer runs were carried out to find out the optimum time interval between volume contractions. Product properties, except those directly related to the problem itself, and drying conditions were maintained invariable throughout the simulation tests to single out

the effect of shrinkage on the computed results The purpose was to reduce computer time as much as possible without compromising the quality of the results

Plots for several shrinkage time steps are presented in Figure 7 10 for comparison As it can be seen from that figure no allowance for volume contraction in the simulation of cacao drying can produce remarkable discrepancies in the predicted results for both product temperature and moisture. On the other hand, there is no need to use a shrinkage time interval of the same order of the time increment required by the numerical procedure For practical purposes shrinkage time steps up to 300 s may be used for cacao A shrinkage time step of 120 s was adopted for this work. Predictions obtained by using this time interval were not much different from those obtained for the time interval of one second

For cacao drying simulations, the time interval chosen is even safer because the actual drying rates are much lower as compared to those of Figure 7 10 The shortest drying test carried out at a temperature of approximately 70 °C took about 13 5 hours to lower the product moisture content from its initial value down to 0 07

Correction for shrinkage was done by regular adjustments of the solution domain after each shrinkage time step The dimensions of the slab were corrected according to the product average moisture content Changes for moisture contents below 0.20 (dry basis) were assumed negligible A shrinking domain results in faster moisture and heat transfers.

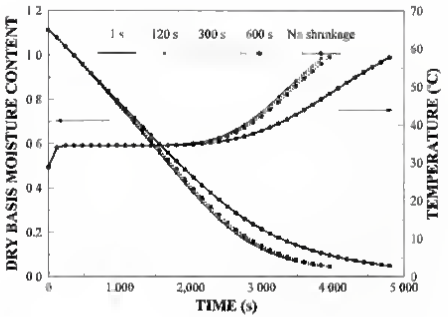


Figure 7 10. Effect of shrinkage time interval on the output of the cacao drying simulation model

Drying Curves

A summary of the drying conditions is given in Table 7 2 The average drying air temperature varied from 40 to about 71 °C, except for tests 07 and 08 which were conducted at 80 °C for reasons to be discussed later The figures presented in Table 7.2 for ambient air temperature and relative humidity are also average values computed over the duration of each test. The complete set of data of moisture loss during the drying experiments is included in Appendix D

Table 7.2. Summary of cacao drying experiments

Test no	Ambient air		Drying air		Moisture content		Test Duration (hour)
	Temp (°C)	RH (%)	Temp (°C)	Velocity (m/s)	Initial (db)	Final (db)	
1	27.1	82.6	70.8	2.58	1.1566	0.0704	13.5
2	29.2	74.1	60.5	2.55	1.1035	0.0760	18.5
3	25.4	89.7	50.8	2.58	1.0665	0.0895	22.5
4	27.7	79.4	40.2	2.56	1.1768	0.0837	42.0
5	29.0	67.9	71.2	2.58	1.1263	0.0636	13.0
6	29.2	72.9	60.0	2.56	1.1584	0.0748	20.5
7	29.0	68.1	49.1	2.56	1.0317	0.0799	28.5
8	28.0	71.4	40.2	2.56	1.1204	0.0885	45.5
9	27.3	77.5	79.7	2.57	1.2386	0.0624	9.5
10	28.3	70.6	79.6	2.58	1.0978	0.0605	10.5
11	26.7	73.0	70.5	1.05	1.2904	0.0653	13.5
12	23.4	69.2	60.6	0.97	1.2247	0.0957	15.5
13	26.8	72.4	50.2	0.99	1.1313	0.0908	24.5
14	27.7	74.4	40.4	1.02	1.2440	0.0902	37.0
15	25.8	83.6	50.0	1.01	1.0986	0.0865	26.0
16	25.3	78.0	40.0	0.97	1.1277	0.0893	43.5
17	27.2	75.7	70.0	1.03	1.0877	0.0570	15.0
18	27.5	73.7	60.1	1.00	1.0513	0.0781	18.0
19	26.7	73.1	70.0	1.01	1.0964	0.0655	14.0
20	25.9	82.3	40.0	0.98	1.0751	0.0858	40.5

Continued

Table 7.2 Continued

Test no	Ambient air		Drying air		Moisture content		Test Duration (hour)
	Temp (°C)	RH (%)	Temp (°C)	Velocity (m/s)	Initial (db)	Final (db)	
21	26 6	78 7	70 0	0 52	1 0825	0 0653	15 0
22	26 4	78 9	50 1	0 48	1 0367	0 0865	28 5
23	26 4	81 9	39 8	0 47	1 0912	0 0941	44 0
24	25 9	75 8	60 0	0 50	1 1409	0 0803	17 5
25	26 5	74 7	70 1	0 55	1 1022	0 0663	14 5
26	25 6	79 3	50 2	0 48	1 3256	0 0949	26 0
27	23 4	77 7	40 1	0 53	1 3318	0 1170	38 5
28	26 4	78 2	60 0	0 55	1 3781	0 0864	20 0
29	24 9	83.2	49 9	0 09	1 1368	0 0765	33 0
30	26 3	78.2	69 9	0 08	1 1988	0 0661	17 5
31	25 5	84 1	50 1	0 11	1 2552	0 0840	33 0
32	26 0	79 2	70 2	0 10	1 3430	0 0583	17 5
33	24 3	82 3	40 1	0 08	1 3262	0 1317	40 0
34	25 2	78 8	60 1	0 12	1 3105	0 0804	23 2
35	25 4	77.3	60 0	0 09	1 3106	0 1043	17 5
36	25 4	78 3	40 0	0 11	1 3160	0 1195	46 8

Actual ambient temperatures and relative humidities changed periodically The former varied within the range of 25 to 32 °C, while the relative humidities varied from 60 to 90%, during the time of execution of the drying experiments Conditions of higher temperatures and lower relative humidities of the ambient air were frequent.

Durations of the drying tests depended on the ambient air conditions, drying temperature, air velocity and product initial and final moisture contents. Initial dry basis moisture content of the samples varied within the range of 1 00 to 1 40. The tests were ended when the final moisture content was in the 0 07-0 10 range. The minimum duration observed was about 15 hours for the highest temperature and air velocity used, about 71 °C and 2 58 m/s, respectively. The maximum duration was about 49 hours for the drying temperature of 40 °C and air velocity of 0 08 m/s.

Experimental results of moisture loss for four preliminary drying tests are plotted in Figure 7 11 for different temperatures. The moisture data were nondimensionalized with respect to the corresponding initial values owing to some variation in the initial moisture content of the samples. A short delay, which may be related to the initial time to heat up the superficial moisture, was observed particularly in those tests carried out at lower temperatures. All curves exhibit a high rate of moisture loss in the initial stages of the drying process. For the highest rate of moisture loss shown, observed for the drying temperature of 70 °C, the sample moisture content was reduced by nearly 50% in an elapsed time of about half an hour. This shows that the amount of moisture loosely bonded to the solids is very significant in fermented cacao beans. This can be verified by examining the initial portions of the curves for elapsed times up to two hours.

Drying rates were computed from the slopes of the drying curves by fitting cubic splines to the experimental data. The slopes of the drying curves of Figure 7 11 are shown in Figure 7 12. The rates of moisture loss varied markedly with the drying temperature. Drying rates dropped sharply as the moisture content of the product reaches

approximately 0 75 From this point onwards, decreases in the rate of drying were relatively lower

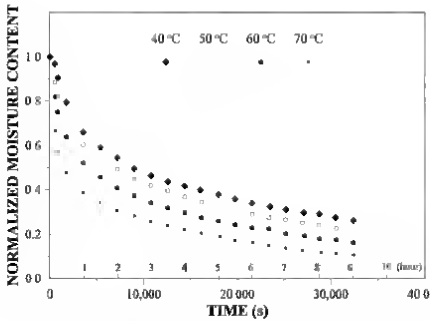


Figure 7.11 Average moisture loss profiles for cacao beans dried at the air velocity of 2 5 m/s

Further analysis of Figure 7 12 shows that periods of constant drying rates seem to have occurred This was more apparent in the tests carried out at lower temperatures The constant rate period seems to be short, however as compared to the duration of the tests It may correspond to evaporation of free water from the external skin of the beans Then the drying rate seems to be controlled by bean shell itself From this stage onwards, although the bean shell was apparently dried out, moisture in liquid form could be

visually observed in the interior of the beans, filling the furrows of the cotyledons, until later stages of the process. Internal liquid moisture could be detected at moisture contents as low as 0 5 to 0 6 This could be easily observed by squeezing partially dried beans (skin dried beans) or by cutting them lengthwise. Below this moisture range, moisture transfer by diffusion within the solid matrix seemed to start to play an important role in the process as the major rate controlling mechanism The drying rate became considerably lower from this point to the end of the process.

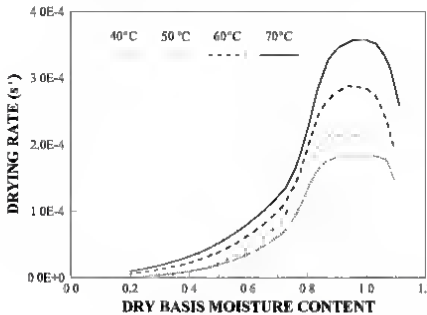


Figure 7.12. Drying rate of fermented cacao beans computed for different drying air temperatures at 2 5 m/s velocity

Constant drying rate periods were much larger in those experiments that combined use of low drying air temperature and velocity. The duration of this drying stage depends on the drying air conditions, such as temperature and relative humidity and velocity. Determination of precise critical moisture content for fermented cacao beans could not be determined under the circumstances of the present work, since the relative humidity of ambient air was not controlled. The solution of the mathematical model allowed for variable boundary conditions, however.

Moisture Diffusity

Moisture diffusivities were estimated from the slopes of the drying curves for the highest value of air velocity (2.5 m/s) at different air temperatures, and corrected by means of the trial-and-error procedure, as explained in the section about mass diffusivity of Chapter 6. The empirical expression of Equation 7.9 was determined by means of linear regression analysis. The determination coefficient (R^2) obtained for the regression equation was 0.8414.

$$D = 9.142 \times 10^{-4} \exp\left(-3.072W + 16.522W^2 - 9.133W^3 - \frac{4565.6}{T}\right) \qquad (7.9)$$

Predictions of moisture diffusivities made with the foregoing expression are shown in Figure 7.13. Plotted diffusivities are effective values computed for bean average moisture content and temperature, since local values for these variables could not be measured. The values of moisture diffusivity estimated varied within the approximate

range of 10^{-11} to 10^{-08} m^2/s, which is comparable to the diffusivities of some grains, with a possible exception for the lower bound of the range. Commercial cacao is dried to a final moisture content (between 7 to 8%, wet basis) much lower than that of other grains.

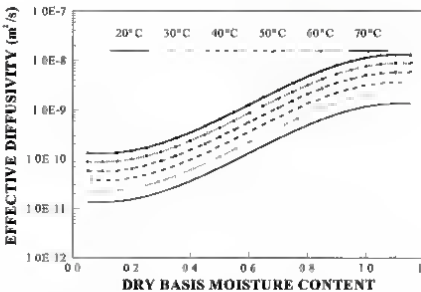


Figure 7.13. Effective moisture diffusivity of fermented cacao beans

Model Validation

The purpose of model validation is to assess the ability of a model to simulate actual processes it was devised to represent. The criterion usually used in situations similar to those of this study consists of measuring the goodness of agreement between predicted results and data collected experimentally

The preliminary simulations carried out with the moisture diffusivity model similar to Equation 7.9, determined using the whole range of cacao moisture content, led to rather poorer predictions. This fact can be appreciated from the plots shown in Figure 7.14. In general, the results, experimental and simulated, differed from each other at greater extent in the initial stages of the drying process and tended to a better agreement towards the end of the tests. At the very beginning, for times less than one hour, the drying model generated over predictions and, then, the converse was observed. The discrepancies achieved values up to 0.15 (dry basis moisture content). The same sort of response pattern from the drying model was verified for lower drying air temperatures and velocities. Figure 7.15 is an example for drying temperature of 40 °C and the same airflow.

The probable explanation, why the outcomes from the simulation runs failed to agree with the experimental data, seems to be associated with the scope of validity of the mathematical expression used to estimate moisture diffusivities from the slope of the experimental drying curves. As already mentioned, the equation referred to above is valid for larger values of time. Another cause, which likely contributed to the source of large errors, is the fact that the equation used can describe moisture transfer under isothermal conditions only. This situation occurs during the initial drying period of cacao beans, when the evaporation rate is high enough to maintain the product temperature constant. This time interval, for the conditions of high airflow used in the experiments designed to determine moisture diffusivity, was shown to be very short in the simulations: less than half an hour, when compared with the total drying time. Besides, this portion of the

drying curve fell below the range of validity of the solution of the mass transfer equation, as discussed previously

Despite the weaknesses of the slope method, its estimates were much closer to the experimental data than those obtained by use of diffusivity models determined for other products In some cases, the results from these attempts did not resemble the expected curves at all The closeness between the results from the slope procedure and the experimental data was very effective, as a starting point, in the process of finding out a better approximations and eventually the best solution as provided by method used

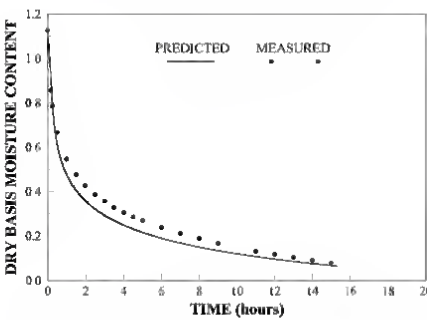


Figure 7.14 Comparison between experimental and preliminary simulated results for cacao dried at 70 °C and 2.5 m/s

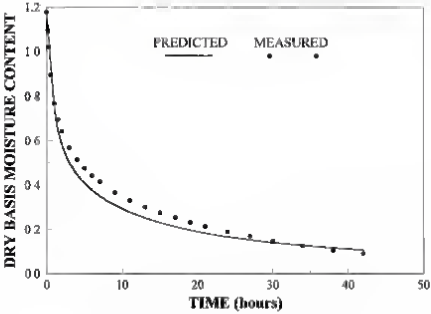


Figure 7-15. Comparison between experimental and preliminary simulated results for cacao dried at 40 °C and 2.5 m/s

Simulation of cacao bean drying using the moisture diffusivity model of Equation 7.9 produce the results shown in Figures 7.16 through 7.22. These graphs are plots of product average moisture content versus time for cacao samples dried at temperatures in the range of 40 to 70 °C. Bean average temperature profiles were also computed, but not used for comparison since no experimental temperature data were collected. The reason for this were the difficulties inherent to temperature measurement in small bodies that experience significant shrinkage during drying.

Comparison between simulated and actual drying data showed that good agreement was achieved. In general, the average differences between simulated and

experimental moisture contents were 0 02 (decimal dry basis) Greater discrepancies were observed at the initial stages of the drying process, for moisture above 0 80, for some experiments carried out at higher air velocities (0 50 1 00 and 2 50 m/s) It took less than one hour to reach 0 80 moisture in these tests For experiments carried out at the lowest air velocity, 0 10 m/s, noticeable differences between predicted and measured values were found up to a moisture content of approximately 0 40 This was more apparent for the lowest drying temperature (40 °C), shown in Figures 7.21 and 7.22

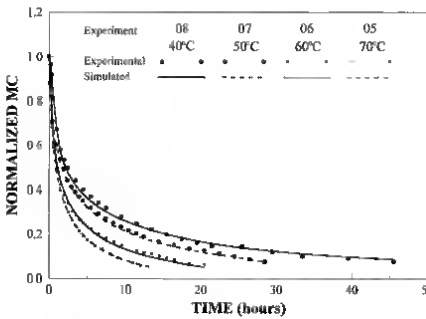


Figure 7.16: Moisture profiles for drying experiments at 2.5 m/s

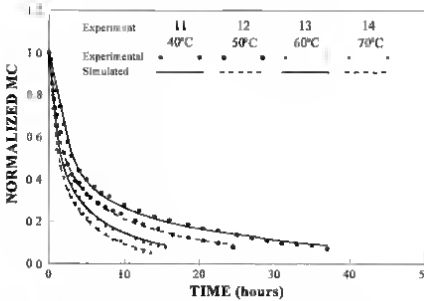


Figure 7.17. Moisture profiles for drying experiments at 1.0 m/s

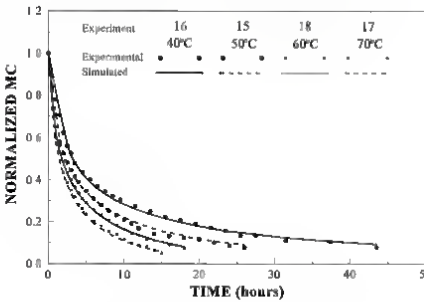


Figure 7.18. Moisture profiles for drying experiments at 1.0 m/s

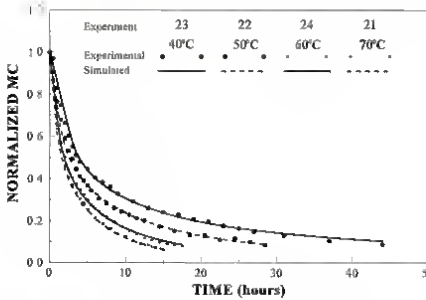


Figure 7.19 Moisture profiles for drying experiments at 0.5 m/s.

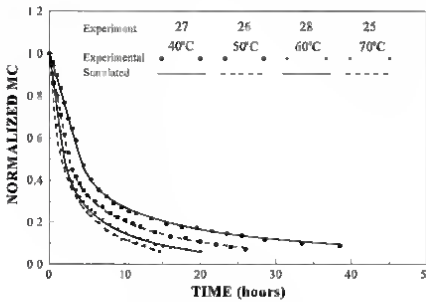


Figure 7.20 Moisture profiles for drying experiments at 0.5 m/s

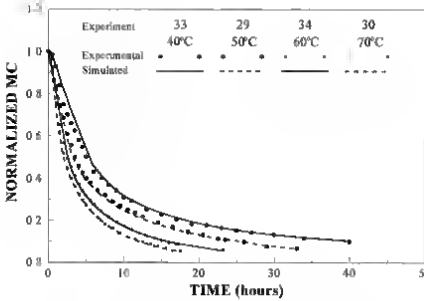


Figure 7.21. Moisture profiles for drying experiments at 0.1 m/s

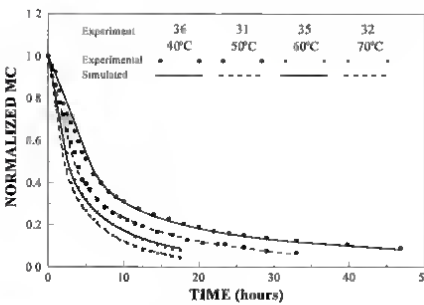


Figure 7.22. Moisture profiles for drying experiments at 0.1 m/s

The probable reason for higher deviations between predicted and experimental results at lower air velocities is the expression used for calculating the convective heat and mass transfer coefficients. The lowest air velocity corresponded to a Reynolds number of about 50.0 that was well below the recommended range of the equation used. These deviations occurred at the initial stage of the drying process, when the transfer rates are greatly controlled by the external resistance to heat and moisture transfer, rather than the internal parameters, the heat and mass diffusivities, which play a more important role towards the end of the process.

Air velocity acts directly on the external resistance to heat and mass transfer. The convective transfer coefficients increases with increasing airflow. As mentioned above, the Reynolds number calculated for the lowest airflow rate was below the range of 500 to 5000. Reynolds number for the air velocity of 0.5 m/s was right below this range, approximately 400, and for 2.5 m/s was about 2000. The heat and the mass transfer coefficients varied within the ranges of 8 to 60 W/m^2 °C and 0.007 to 0.060 kg/m^2 s, respectively. Figure 7.23 shows the variation of the heat and mass transfer coefficients with air velocity of a typical slab size of 24x14x7 mm.

Temperature Profiles

Computed average product temperature profiles, for some of the experiments, are presented in Figures 7.24 and 7.25. These profiles also show that the bean samples experienced a short warming up period at the very beginning of the drying process. Then a period of nearly constant temperature followed. The length of this period depended on

the drying air temperature and velocity Shorter periods of low temperature were associated with drying conditions of high air temperatures and velocities, and vice-versa.

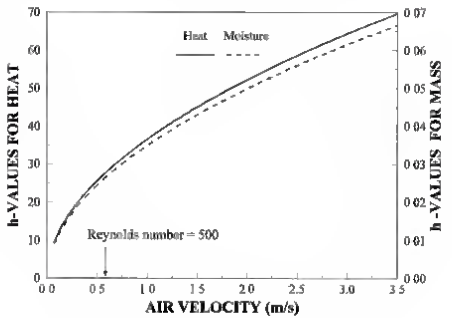


Figure 7.23. Convective transfer coefficients (h values) for heat (W/m^2 °C) and mass (kg/m^2 s)

Although sample temperatures were not measured in the drying tests for comparison purposes, the cooling effect, resultant from evaporation of free moisture, could be sensed at the beginning of each run The exhaust air from the drier, after passing through the drying tray, remained at relatively lower temperatures than the incoming air, for a length of time that varied with the drying. This effect was observed while liquid moisture could be viewed on the mucilaginous surface of the cacao beans

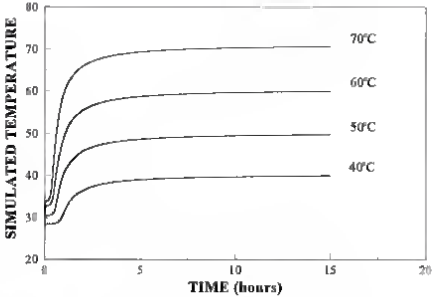


Figure 7.24. Average temperature profiles for air velocity of 2.5 m/s

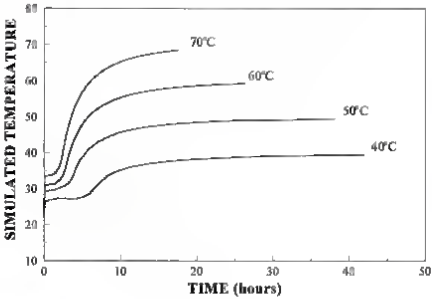


Figure 7.25. Average temperature profiles for air velocity of 0 5 m/s

After the simulated product temperature started rising it approached the drying air temperature quite fast for higher air velocities. This is plausible due to the high value of the convective heat transfer coefficient. For lower airflows this phenomena took longer, as expected

Effect of Ambient Air Relative Humidity

Relative humidity affects the external potential that drives off moisture from the product in contact with the air. The product equilibrium moisture content is a function of both air temperature and relative humidity. The former could be controlled and was maintained constant during the drying tests. The relative humidity of the drying air varied with that of the ambient

In order to have an appraisal of the effect of this variable on the output of the drying model, some simulations were carried out at constant, equal to the average calculated for the drying test, and variable relative humidity. In this case the values monitored in the course of the corresponding experiment were used as input to the computer program. Comparison was made by contrasting the simulated results shown in Figure 7.26. The maximum deviation in moisture content verified for this case was 0.015 (decimal dry basis). The curves obtained for temperature presented more noticeable deviations. The maximum difference that was observed for the temperature profiles was about 5.6 °C. Both occurred at the initial phase of the process, possibly in the constant drying rate period.

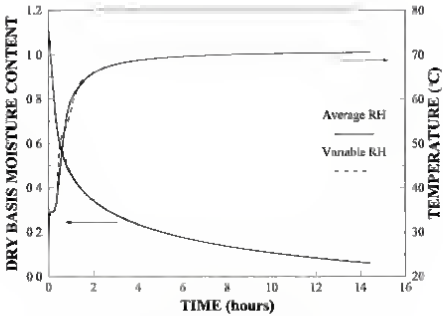


Figure 7.26. Simulation of drying test at average and variable ambient relative humidity (RH) and air velocity of 2.5 m/s

Product Acidity

Acidity in fermented cacao results from the presence of several organic acids both volatile and non-volatile. Acetic acid is the most important volatile acid. It is formed during the fermentation process. Lactic and citric acids may be considered as the most important non-volatile acids. The former is produced in the course of the fermentation process, whereas citric acid occurs naturally in the pulp of fresh cacao. This acid is partially used up during fermentation. Both types of acids are important for their role in

determining certain aspects of the flavor of cacao end products However, lactic and acetic acids probably play the most important roles concerning the acidic taste in chocolate Higher residual concentrations of these compounds in the dried beans usually lead to a sour end product, while the presence of acids in smaller quantities may contribute to the fruity/floral flavor characteristic of the chocolate obtained from some types of cacao By being a volatile constituent acetic acid may be lost in several stages of the primary and final processing of cacao These phases include fermentation itself, drying, roasting and other heat treatments of the manufacturing process

The results obtained in the experiments on drying of cacao, under thin layer conditions, are shown in Figure 7 27 through 7 30 In these graphs, acid contents, expressed in terms of mass of acid per unit mass of dry solids are plotted against time for the drying experiments at 2 5 m/s and temperatures in the range of 40 to 70 °C The data points presented were actually averages of three readings

There was no detectable decrease in acetic acid concentration in the course of the drying tests There were some small fluctuations among the readings from the chromatographer Acetic acid seemed to have a behavior similar to those of the other acids used for comparison, namely lactic and citric acids, which are sometimes referred to as fixed acids The acid concentrations were about 0 02 0 01 and less than 0 05 for acetic lactic and citric acids, respectively These concentrations are comparable to some data available for Bahian cacao in the literature (Lopez, 1983) The same pattern was observed for air velocities of 0 1, 0 5 and 1 0 m/s The concentrations of acetic acid achieved the highest values, followed by those of lactic and citric acid (Appendix B)

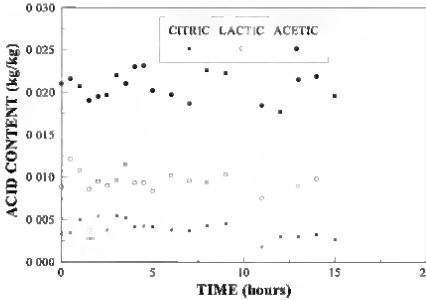


Figure 7.27. Acid concentration profiles for cacao dried at 70 °C and 2.5 m/s

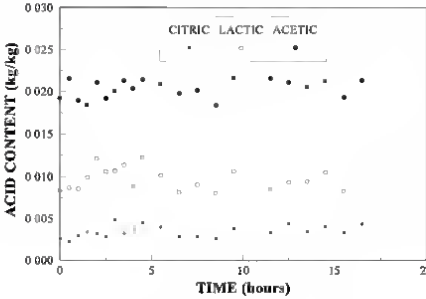


Figure 7.28. Acid concentration profiles for cacao dried at 60 °C and 2.5 m/s

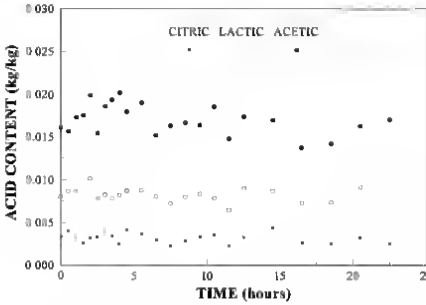


Figure 7.29 Acid concentration profiles for cacao dried at 50 °C and 2.5 m/s

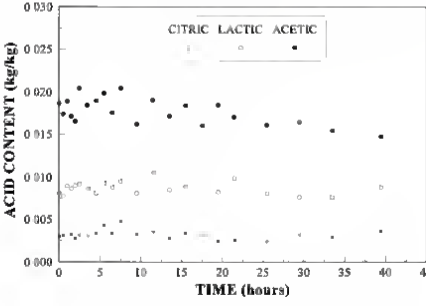


Figure 7.30 Acid concentration profiles for cacao dried at 40 °C and 2.5 m/s

Two drying tests were carried out at 80 °C to further explore the possibility of any success in removing acetic acid by increasing the drying air temperature Acetic acid concentration remained nearly constant throughout the drying process as illustrated by Figure 7 31 Higher temperatures were not tried due to limitations of the equipment used

The acetic acid concentration in the 80 °C test of Figure 7 31 was somewhat lower than those of the previous experiments. This was due to the difference in the amount of liquid in the incoming fresh cacao pulp Higher quantity of liquid pulp tends to limit aeration by obstruction of the interstitial spaces in the fermentation box As a consequence, the fermented product may exhibit higher concentrations of lactic and acetic acids. The converse results in better aeration and a less acidic fermented product.

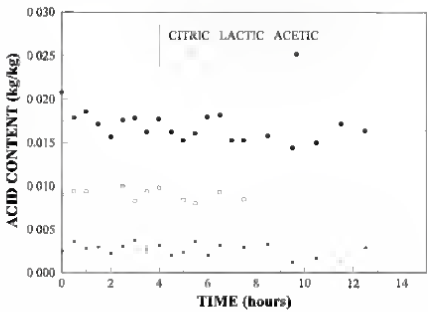


Figure 7.31 Acid concentration profiles for cacao dried at 80 °C and 2 5 m/s

The results obtained in this work may appear to be in conflict with some findings reported in the cacao literature. There have been reports that sun drying (Duncan et al., 1989) and slower deep bed drying at 40-45 °C (Dias and Avila, 1993) removed acetic acid during the drying process. However, the drying conditions of this project are quite different from what have been done in the past, even though the range of temperatures may be similar.

Sun drying is a very slow process allowing time for the decomposition and migration of acetic acid while the product remains wet. The low temperature artificial drying that resulted in some loss of acetic acid were carried out in thick beds, 0.1 to 0.25 m deep. In thick bed drying, the product experiences conditions completely different from those found in its counterpart, thin layer drying or drying under fully exposed conditions. In thick bed drying, not all the beans are subjected to the same conditions of the inlet air, during all the process duration. In thin layer drying, the beans lose moisture at a much higher rate than the average drying rate of thick bed under the same conditions of air temperature and air velocity.

Roasting of commercial beans, in thin layers, at air temperatures of 150 °C for about 30 minutes was effective in reducing the acetic acid content of the samples by as much as 22% of its initial content (Jinap and Dimick, 1991). Even higher reductions in acidity, up to 40%, have been reported in the literature surveyed by these authors. Consequently, it appears that removal of acetic acid from fermented beans is a physical process highly intensive in terms of energy requirements. It appears that temperature is the critical factor in acetic removal rather than exposure time.

It may be inferred from Jinap and Dimick's work on bean roasting that the argument of insufficient time for acetic acid to migrate from the interior of the beans to their exterior is somewhat weak. The strength with which acetic acid molecules are bonded to the cacao bean solid matrix seems to be much higher than that of water. These bonds may be broken only under temperatures used in bean roasting. However, if the drying is done at very high temperatures the dried cacao would suffer some major and undesirable consequences related to the progression of the flavor precursor forming chemical reactions. Determination of the equilibrium relationship between vapor pressure of acetic acid and its concentration in the beans at different moisture contents and temperatures may elucidate this problem.

CHAPTER 8
CONCLUSIONS

Based on the experimental and drying simulation results obtained during the execution of this work the following conclusions may be drawn from this study:

1 Cacao undergoes considerable shrinkage during the drying process. Change in size, expressed by changes in the dimensions of the beans, depends on direction. Accommodation of the swollen cotyledons during drying accounts for most of the size changes, rather than shrinkage caused by the hygroscopic behavior of the product itself.

2 The total heat of moisture vaporization is an important property in the study of cacao drying, owing to the fact that cacao has to be dried to fairly low moisture content, in the range of 7 to 8% (wet basis) for safe storage.

3 A mathematical model was developed to relate moisture diffusivity of fermented cacao beans to changes in product average moisture content and temperature during drying.

4 The drying model developed to simulate the drying process of fully exposed fermented cacao beans proved to be effective since it could generate good predictions of average moisture changes during the process.

5. Bean volume reduction has significant effect on the results predicted with the simulation model for moisture loss. Models that do not account for the effect of this parameter may not be suitable for use with fermented cacao.

6 Although acetic acid is a volatile compound, it is not possible to remove perceptible quantities in the drying process carried out under recommended conditions of temperature (no higher than 70 °C). This compound, which is absorbed by the beans in the fermentation stage, has a similar behavior to those of citric and lactic acids, which are considered as fixed acids. Therefore, artificial drying does not contribute to improve product quality by reducing its acidity.

It is claimed in the literature that the fermentation process of cacao reduces the barrier imposed by the bean shell to moisture loss during drying. This particular component seems to have an important role in controlling the rate of moisture loss in the drying process, after the skin-dried stage is attained. Therefore, it is recommended that future research works should concentrate efforts to measure moisture diffusivities for the bean hull and cotyledons individually.

APPENDIX A
CONSTITUTIVE EQUATIONS

In an ideal situation the transport phenomena that take place in hygroscopic and porous media may be considered as isolated or independent events, that is, as noninteracting phenomena. Therefore it can be said that the rate of flow of a component is a function of the gradient of the corresponding driving force or field potential variable only This statement may be written in functional form as

$$\mathbf{J} = \mathbf{J}(\mathbf{X}) \qquad \textbf{(A.1)}$$

The expression above may be expanded about the condition of equilibrium (X=0) using Taylor series to yield

$$J = J(X=0) + \frac{\partial J(X)}{\partial X}\Delta X + \frac{1}{2!}\frac{\partial^2 J(X)}{\partial X^2}(\Delta X)^2 + \ldots \qquad \textbf{(A.2)}$$

Equation A.2 may be simplified for conditions of local equilibrium or microscopic reversibilities This implies that the rate of a biased movement is small compared to normal fluctuations (Forland et al , 1988) Therefore, for slow processes and small departures from equilibrium, the higher order terms of the series above may be dropped off This leads to a simple linear relationship between a flow and its driving force of the form

$$\mathbf{J} = L\mathbf{X} \qquad \textbf{(A.3)}$$

Every day experience has shown that this type of relationship is valid for a large class of irreversible phenomena and for wide ranges of experimental conditions (Mikhailov and Ozisik, 1983). Instances of this expression may be given by Fourier and Fick's laws of heat and mass transfer, respectively. Equations of this kind are empirical and generalized evidence (Morowitz, 1970). They are also considered assumptions of a theory (Stanislav, 1982). The coefficient L may be interpreted as generalized conductance or mobility (Katchalsky and Curran, 1967).

For multicomponent systems with interactive forces and fluxes, the relationships between causes and effects may be given by a set of mathematical equations as follows

$$\mathbf{J}_i = \mathbf{J}_i(\mathbf{X}_j) \tag{A.4}$$

or

$$\mathbf{X}_i = \mathbf{X}_i(\mathbf{J}_j) \tag{A.5}$$

for i and j=1, 2,

Reasoning similar to the one employed for independent flows or single component systems may be followed through for multicomponent systems. By using the same assumptions, a set of linear relationships, called phenomenological equations, may be derived (Wisniewski et al., 1976). Employing the summation convention, these relationships may be expressed as in Equation A.6

$$\mathbf{J}_i = L_{ij}\mathbf{X}_j \tag{A.6}$$

Coefficients with the same indices ($i=j$) are straight or direct coefficients that relate conjugated forces and generalized fluxes That is, these coefficients associate fluxes to their main driving forces. Whilst those with differing indices ($i \neq j$), the cross coefficients, couple interactive nonconjugated forces and fluxes. They actually combine cross effects, that is they account for interfering influences of forces that act directly upon other flows These coefficients may have important contribution to the total flow or not. Equation A 6 shows that any flux is given in terms of a linear combination of the interacting forces.

Mathematical expressions for the driving forces, as functions of physically interpretative variables may be derived from the entropy production function. It is required to perform some manipulations and to account for the underlying assumptions it is subject to This equation may be further modified to yield the dissipation function Both may be obtained from the combination of the first and second principles of thermodynamics for an open system or control volume. They can also be interpreted in terms of products of forces (variations of thermodynamic functions) and fluxes (quantities to be transferred). If flows and forces are properly chosen from the entropy production (Equation A 7) or dissipation function (Equation A 8) the matrix of coefficients L is symmetric

$$\sigma = -\mathbf{J}_q \nabla\left(\frac{1}{T}\right) - \sum_{i=1}^{n}\left(\frac{\mathbf{J}_i}{T}\right)\nabla\mu_i \qquad \text{(A.7)}$$

$$\Psi = -\mathbf{J}_q \nabla\left(\frac{1}{T}\right) - \sum_{i=1}^{n}\mathbf{J}_i \nabla\mu_i \qquad \text{(A.8)}$$

Furthermore, the choice of the thermodynamic components on the ground of the Gibbs Phase Rule can guarantee the independence of forces (Forland et al , 1988) These expressions are bilinear of generalized fluxes and their conjugated forces And they establish the basis for expressing for flows and fluxes in mathematical terms.

APPENDIX B
BALANCE EQUATIONS

Mathematical Description of a Flow Field

Transport phenomena taking place in multicomponent material media can be described by means of balance equations for extensive quantities. The intensive properties that characterize the local state of the components appear in these equations. These quantities depend on position and time. Therefore, an arbitrary function or property φ of the flow may be represented as

$$\varphi = \varphi(x, y, z, t) \tag{B 1}$$

The position functions x, y and z depend on time t only. The total differential of φ at a point can be obtained as follows

$$d\varphi = \frac{\partial \varphi}{\partial x} dx + \frac{\partial \varphi}{\partial y} dy + \frac{\partial \varphi}{\partial z} dz + \frac{\partial \varphi}{\partial t} dt \tag{B.2}$$

Application of the chain rule of differentiation for composite functions yields the following expression (Kaplan, 1991, Lang, 1994)

$$\frac{d}{dt}(\varphi) = \frac{\partial \varphi}{\partial x}\frac{dx}{dt} + \frac{\partial \varphi}{\partial y}\frac{dy}{dt} + \frac{\partial \varphi}{\partial z}\frac{dz}{dt} + \frac{\partial \varphi}{\partial t} \tag{B.3}$$

This total time derivative has different meanings depending on the frame of reference (Wisniewski et al , 1976) For a fixed frame the positional variables do not change with respect to time, thus the total and the partial time derivatives are equal

$$\frac{d}{dt}(\varphi) = \frac{\partial \varphi}{\partial t} \tag{B.4}$$

If the reference frame is attached to the material particle and moves or is convected with the flow then the partial derivatives of the functions of position represent the velocity of the material particle with respect to a second and fixed frame. The total derivative is also called substantial derivative (Bird et al , 1960). Yet material or convective derivative (Aris, 1962)

$$\frac{d}{dt}(\varphi) = \frac{\partial \varphi}{\partial x} v_x + \frac{\partial \varphi}{\partial y} v_y \frac{\partial \varphi}{\partial z} v_z + \frac{\partial \varphi}{\partial t}$$

or (B.5)

$$\frac{d}{dt}(\varphi) = \mathbf{v} \cdot \nabla \varphi + \frac{\partial \varphi}{\partial t}$$

Generalized Balance Equation for Homogeneous Control Volume

A material particle moving throughout a flow field may be represented by a small volume element (dV) as portrayed in Figure B 1. The particle has an initial position $\mathbf{x}_o$ and then it is displaced and takes on a new configuration or position $\mathbf{x}$ at time t Therefore, the actual particle position is a function of its initial location and time.

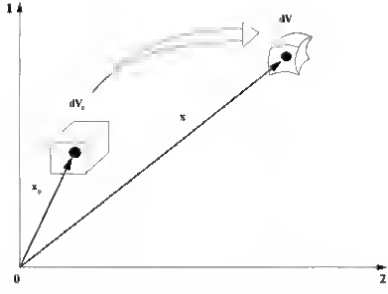


Figure B 1. Schematic representation of dilatation in a flow field

The element volume may be distorted. Yet, it may undergo expansion or shrinkage along its path, while its integrity is preserved since the flow is continuous. The flow field as represented can be described by a point transformation (Aris, 1962)

Considering the following notation for the element volume:

1 Position vector
$\mathbf{x}_o$ at time $t = 0$
at time t

$$\mathbf{x} = \mathbf{x}(\mathbf{x}_o, t) \qquad \textbf{(B 6)}$$

2 Material particle (element volume)
dV_o at time $t = 0$
dV at time t

$$dV_o = \mathbf{dx}_o . \mathbf{dy}_o \times \mathbf{dz}_o \quad \text{and} \quad dV = \mathbf{dx} . \mathbf{dy} \times \mathbf{dz} \tag{B.7}$$

3 Velocity vector

$\mathbf{v}_o$ at time $t = 0$

at time t

$$\mathbf{v} = \mathbf{v}(\mathbf{v}_o, t) \tag{B.8}$$

4 Gradient operator

$$\nabla = \frac{\partial}{x}\mathbf{i} + \frac{\partial}{y}\mathbf{j} + \frac{\partial}{z}\mathbf{k} \tag{B.9}$$

5 Jacobian

$$J = \frac{\partial (x, y, z)}{\partial (x_o, y_o, z_o)} = \frac{dV}{dV_o} \tag{B.10}$$

6 Divergence

$$\text{div}\,\mathbf{v} = \frac{1}{J}\frac{\partial J}{\partial t} \tag{B 11}$$

The control volume depicted in Figure B 2 illustrates a heterogeneous material body. The total volume of material (V), which includes regions 1 and 2, is confined by the external surface (S). The body experiences changes in shape and size such that its surrounding surface moves with velocity **v** either inwards due to shrinkage, or outward, due to expansion, or yet with the bulk of fluid. The symbol **n** is the outward normal unit vector to the body surface.

The front, represented by surface Σ, also moves, receding or advancing, with an arbitrary velocity **u**. This surface represents a singular interface (Slattery, 1967). At this surface jump conditions or discontinuities may arise (Taylor and Krishna, 1993). An

arbitrary variable may or may not suffer discontinuity across this interface Phase change of a component of the medium is a typical example of discontinuity In this case a variable under observation takes different limiting values on either of its sides. The outward normal unit vector to Σ is represented by v

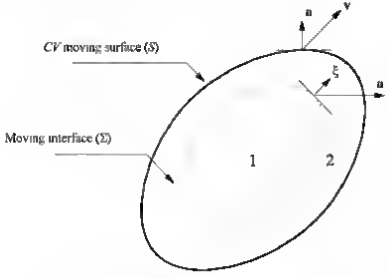


Figure B.2. Pictorial representation of a control volume showing an interface of discontinuity - phase change

A homogeneous region may be visualized by ignoring the presence of a jump interface in Figure B.2, that is, by considering the total volume of the region bounded by surface (S) Any intensive quantity can be represented by a continuous field function $f(\mathbf{x},t)$ The mass density or concentration of the material (ρ) also varies with position and time The total amount (F) of this quantity contained in the volume domain is obtained by

integrating this function over $V(t)$ It represents the corresponding extensive property and it is a function of time only as in Equation B 12

$$F(t) = \iiint_{V(t)} \rho f(\mathbf{x},t)\,dV \qquad \textbf{(B 12)}$$

Balance equations are expressed in terms of time rates of change Thus, the total or material time derivative of the expression above has to be derived from

$$\frac{d}{dt}[F(t)] = \frac{d}{dt}\iiint_{V(t)} \rho f\,dV \qquad \textbf{(B.13)}$$

Since the domain of Equation B 12 depends on time, the differentiation above (Equation B.13) can not be worked out without performing transformation of coordinates (Kaplan, 1991) Thus, by changing coordinates, Equation B.12 becomes

$$F(t) = \iiint_{V_o} \rho f(\mathbf{x},t)\left(\frac{dV}{dV_o}\right)dV_o \qquad \textbf{(B 14)}$$

On substitution for the new expression for $F(t)$, use of the Leibnitz's rule of integration and carrying out the required manipulations Equation B 15 is obtained (Kaplan, 1991) This sequence of operations is known in the literature as the Reynolds transport theorem (Aris, 1962).

$$\frac{d}{dt}[F(t)] = \iiint_{V(t)} \left\{\frac{\partial}{\partial t}(\rho f) + \nabla.[(\rho f)\mathbf{v}_c]\right\}dV \qquad \textbf{(B 15)}$$

Applying the divergence theorem to the integrand on the left hand side of Equation B 16 yields the following

$$\frac{d}{dt}\left[\iiint_{V(t)} F(t)\,dV\right] = \iiint_{V(t)} \frac{\partial(\rho f)}{\partial t}\,dV + \iint_{S(t)} (\rho f)\,\mathbf{v}_s \cdot \mathbf{n}\,dS \qquad \textbf{(B 16)}$$

Equation B 16 renders prompt physical meaning. It may be inferred from this expression that the rate of change of the integral of an arbitrary field variable within a moving control volume is equal to the integral of the local rate of change added by the net flow across the volume surface. Flow through the system boundary may occur by advection or molecular diffusion. Generation or depletion of matter may also occur within the volume, but this is not considered here.

Generalized Balance Equation for Heterogeneous Control Volume

A heterogeneous system may consist of two or more phases. The volume of Figure B 2 satisfies this condition such that the following may apply:

1 Total volume

$$V(t) = V_1(t) + V_2(t) \qquad \textbf{(B 17)}$$

2 Phase interface orientations

$$\xi_1 + \xi_2 = 0 \qquad \textbf{(B 18)}$$

In accordance with Equation B 17, the integration of the time varying extensive quantity F over the whole volume (Equation B 12) may be split into two integrals over each of the subvolumes (Lang, 1994) to yield

$$F(t) = \iiint_{V_1(t)} (\rho f)\,dV + \iiint_{V_2(t)} (\rho f)\,dV = \sum_{i=1}^{2} \left[\iiint_{V_i(t)} (\rho f)\,dV \right] \qquad \text{(B 19)}$$

The same applies to the time derivative

$$\frac{d}{dt}[F(t)] = \underbrace{\frac{d}{dt}\left[\iiint_{V_1(t)} (\rho f)\,dV \right]}_{\mathbf{I}} + \underbrace{\frac{d}{dt}\left[\iiint_{V_2(t)} (\rho f)\,dV \right]}_{\mathbf{II}} \qquad \text{(B.20)}$$

The time derivatives may be carried out by applying the Reynolds transport theorem to the terms **I** and **II** in the above expression

1 Volume I

$$\frac{d}{dt} \iiint_{V_1(t)} (\rho f)\,dV = \iiint_{V_1(t)} \frac{\partial (\rho f)}{\partial t}\,dV + \iint_{\Sigma(t)} (\rho f)_1 (\mathbf{u}_{\cdot} \xi_1)\,dA \qquad \text{(B.21)}$$

2 Volume II

$$\frac{d}{dt} \iiint_{V_2(t)} (\rho f)\,dV = \iiint_{V_2(t)} \frac{\partial (\rho f)}{\partial t}\,dV + \iint_{S(t)} (\rho f)\,(\mathbf{v}_s \cdot \mathbf{n})\,dA + \iint_{\Sigma(t)} (\rho f)_2 (\mathbf{u}_{\cdot} \xi_2)\,dA \qquad \text{(B.22)}$$

$(\rho f)_1$ and $(\rho f)_2$ are limiting values associated with any point that approaches another point on the singular surface from V_1 and V_2, respectively

Addition of the integrals for volumes **I** and **II** results in the expression

$$\frac{d}{dt} \iiint_{V(t)} (\rho f)\,dV = \iiint_{V(t)} \frac{\partial (\rho f)}{\partial t}\,dV + \iint_{S(t)} (\rho f)\,(\mathbf{v}_s \cdot \mathbf{n})\,dA + \iint_{\Sigma(t)} \left[\sum_{i=1}^{2} (\rho f)(\mathbf{u}_{\cdot} \xi_i) \right] dA \qquad \text{(B.23)}$$

Interpretation of this total differential is similar to that for homogeneous system The third term on the right hand side of Equation B 23 accounts for the transfer rates across the phase change or jump interface (Σ)

From Equation B 23 the following interpretations may apply to any arbitrary variable

1 "Jump ' operator

$$\sum_{i=1}^{n}\left[\alpha(\mathbf{X}.\xi)\right]_i=\alpha_1(\mathbf{X}_1.\xi_1)+\alpha_2(\mathbf{X}_2.\xi_2)+... \qquad \textbf{(B.24)}$$

2. "Jump" form of the divergence theorem,

$$\iiint_V \nabla.\mathbf{X}\,dV = \iint_S \mathbf{X}.\mathbf{n}\,dA + \iint_\Sigma \left[\sum_{i=1}^{n}(\mathbf{X}.\xi)\right]dA \qquad \textbf{(B.25)}$$

Conservation of Mass

The law of conservation of mass for a substance occupying an arbitrary volume can be stated as

$$\begin{pmatrix} rate\ of \\ accumulation \\ within\ the\ CV \end{pmatrix} = \begin{pmatrix} net\ rate\ of \\ transport \\ across\ S \end{pmatrix} + \begin{pmatrix} net\ rate\ of \\ generation/depletion \\ within\ the\ CV \end{pmatrix} \qquad \textbf{(B 26)}$$

Assuming that there is no generation or depletion of mass, then the rate of accumulation is given by Equation B 27 This conservation equation is expressed in terms of the material velocity relative to that of the external surface velocity (Bird et al , 1960; Standart, 1964) Applying Equation B.23 with $f = 1$

$$\frac{d}{dt}\iiint_{V(t)}(\rho)dV = \iiint_{V(t)}\frac{\partial(\rho)}{\partial t}dV + \iint_{S(t)}(\rho)(\mathbf{v}_s.\mathbf{n})dA + \iint_{\Sigma(t)}\left[\sum_{i=1}^{2}(\rho)(\mathbf{u}.\xi_i)\right]dA \qquad \textbf{(B.27)}$$

Use of the divergence theorem of Equation B 25 for $\mathbf{X} = \rho v$ to transform the second term on the left of the foregoing expression leads to

$$\iiint_{V(t)} \nabla.(\rho \mathbf{v}) dV = \iint_{S(t)} (\rho \mathbf{v}).\mathbf{n} dA + \iint_{\Sigma(t)} \left[\sum_{i=1}^{2} (\rho \mathbf{v}.\xi) \right] dA \qquad \textbf{(B.28)}$$

Rearranging Equations 27, 28 and 29, the following expression is obtained

$$\iiint_{V(t)} \left[\frac{\partial \rho}{\partial t} + \nabla.(\rho \mathbf{v}) \right] dV = \iint_{\Sigma(t)} \left[\sum_{i=1}^{2} \rho(\mathbf{v} - \mathbf{v}_b).\xi \right] dA \qquad \textbf{(B.29)}$$

The integrands of the expression above must vanish everywhere For each phase the local differential form of the equation of continuity is obtained

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho \mathbf{v}) = 0 \qquad \textbf{(B.30)}$$

At the phase interface the following flux jump condition applies

$$\sum_{i=1}^{2} \rho(\mathbf{v} - \mathbf{v}_b).\xi = 0 \qquad \textbf{(B.31)}$$

Similar steps may be followed for individual constituents of a mixture Thus for $f = \rho_i / \rho$ and $\mathbf{X} = \rho_i \mathbf{v}_i$ the following may be obtained for each phase

$$\frac{\partial \rho_i}{\partial t} + \nabla.(\rho_i \mathbf{v}_i) = 0 \qquad \textbf{(B.32)}$$

and for the phase interface the flow relationship is given by

$$\sum_{i=1}^{2} \rho_i (\mathbf{v}_i - \mathbf{v}_b).\xi = 0 \qquad \textbf{(B.33)}$$

APPENDIX C
BASIC MASS TRANSFER RELATIONSHIPS

Concentration Relationships

Arbitrary System

Species identification (i)
Total volume of the system (V)
Number of species in the mixture (n)
Total mass in the system

$$m = m_1 + m_2 + m_3 + \quad \text{(C 1)}$$

Mass density

$$\rho = m/V \quad \text{(C.2)}$$

Concentration of species

$$\rho_i = m_i/V \quad \text{(C.3)}$$

$$\rho = \rho_1 + \rho_2 + \rho_3 + \quad \text{(C.4)}$$

Mass fraction of species

$$\omega_i = \rho_i/\rho \quad \text{(C.5)}$$

$$\omega_1 + \omega_2 + \omega_3 + = 1 \quad \text{(C 6)}$$

Mass ratio of species

$$\gamma_i = \frac{\omega_i}{1-\omega_i} = \frac{\rho_i}{\rho - \rho_i} = \frac{\rho_i}{\rho_s} \qquad \text{(C.7)}$$

Cacao Bean

Component 1 - acetic acid (a)
Component 2 - moisture (w, water)
Component 3 - dry bone mass (s, dry solids)
Total mass of wet bean

$$m = m_a + m_w + m_s \qquad \text{(C.8)}$$

Mass concentration

Acetic acid

$$C_a = m_a / V \qquad \text{(C.9)}$$

Moisture

$$C_w = m_w / V \qquad \text{(C.10)}$$

Dry bone material

$$C_s = m_s / V \qquad \text{(C.11)}$$

Bean mass density

$$\rho = C_a + C_w + C_s \qquad \text{(C.12)}$$

Mass fraction (wb wet basis)

Acetic acid

$$A_{wb} = m_a / m \qquad \text{(C.13)}$$

Moisture

$$W_{wb} = m_w / m \qquad \text{(C.14)}$$

Solids

$$S_{wb} = m_s / m \tag{C.15}$$

$$A_{wb} + W_{wb} + S_{wb} = 1 \tag{C.16}$$

Mass ratio (*db*, dry basis)

Acetic acid

$$A_{db} = m_a / m_s \tag{C.17}$$

Moisture

$$W_{db} = m_w / m_s \tag{C.18}$$

Dry solids

$$S_{db} = m_s / m_s = 1 \tag{C.19}$$

$$A_{db} + W_{db} + S_{db} \geq 1 \tag{C.20}$$

Relationships between concentration and mass fraction

Acetic acid

$$C_a = \frac{m_a}{V} = \frac{m_a / m}{V / m} = \frac{A_{wb}}{1/\rho} = \rho A_{wb} \tag{C.21}$$

Moisture

$$C_w = \frac{m_w}{V} = \frac{m_w / m}{V / m} = \frac{W_{wb}}{1/\rho} = \rho W_{wb} \tag{C.22}$$

Solids

$$C_s = \frac{m_s}{V} = \frac{m_s / m}{V / m} = \frac{S_{wb}}{1/\rho} = \rho S_{wb} \tag{C.23}$$

Relationships between concentration and mass ratio

Acetic acid

$$C_a = \frac{m_a}{V} = \frac{m_a/m_s}{V/m_s} = \frac{A_{ab}}{1/\rho_a} = \rho_s A_{ab} \qquad \textbf{(C 24)}$$

Moisture

$$C_w = \frac{m_w}{V} = \frac{m_w/m_s}{V/m_s} = \frac{W_{db}}{1/\rho_a} = \rho_s W_{db} \qquad \textbf{(C.25)}$$

Solids

$$C_s = \frac{m_s}{V} = \frac{m_s/m_a}{V/m_a} = \frac{1}{1/\rho_a} = \rho_a \qquad \textbf{(C.26)}$$

Relations between mass fraction and mass ratio

Acetic acid

$$A_{wb} = \frac{m_a}{m} = \frac{m_a}{m_a + m_w + m_s} = \frac{m_a/m_s}{m_a/m_s + m_w/m_s + 1} = \frac{A_{db}}{A_{db} + W_{db} + 1} \qquad \textbf{(C.27)}$$

$$A_{db} = \frac{m_a}{m_s} = \frac{m_a}{m - m_a - m_w} = \frac{m_a/m}{1 - m_a/m - m_w/m} = \frac{A_{wb}}{1 - A_{wb} - W_{wb}} \qquad \textbf{(C.28)}$$

Moisture

$$W_{wb} = \frac{m_w}{m} = \frac{m_w}{m_a + m_w + m_s} = \frac{m_w/m_s}{m_a/m_s + m_w/m_s + 1} = \frac{W_{db}}{A_{db} + W_{db} + 1} \qquad \textbf{(C.29)}$$

$$W_{db} = \frac{m_w}{m_s} = \frac{m_w}{m - m_a - m_w} = \frac{m_w/m}{1 - m_a/m - m_w/m} = \frac{W_{wb}}{1 - A_{db} - W_{db}} \qquad \textbf{(C.30)}$$

Dry solids

$$DS_{wb} = \frac{m_a}{m} = \frac{m_a}{m_a + m_w + m_s} = \frac{1}{m_a/m_s + m_w/m_s + 1} = \frac{1}{A_{db} + W_{db} + 1} \qquad \textbf{(C.31)}$$

$$DS_{db} = \frac{m_s}{m_s} = \frac{m_s}{m - m_a - m_w} = \frac{m_s/m}{1 - m_a/m - m_w/m} = \frac{S_{wb}}{1 - A_{db} - W_{db}} \qquad \textbf{(C.32)}$$

Flux Relationships

Arbitrary System

Directed external surface (**A**)
Velocity of species

$$\mathbf{U}_i = \frac{\Delta \mathbf{x}}{\Delta t} \tag{C.33}$$

Mass flow of species

$$\dot{m}_i = \frac{\Delta m_i}{\Delta t} \tag{C.34}$$

Flux in terms of mass concentration

$$\mathbf{n}_i = \frac{\dot{m}_i}{\Delta \mathbf{A}} = \frac{m_i}{\Delta \mathbf{A}} \frac{\Delta \mathbf{x}}{\Delta t} = \frac{\Delta m_i}{\Delta \mathbf{A} \Delta \mathbf{x}} \frac{\Delta \mathbf{x}}{\Delta t} = \frac{\Delta m_i}{\Delta V} \mathbf{U}_i = C_i \mathbf{U}_i \tag{C.35}$$

Flux in terms of mass fraction

$$\mathbf{n}_i = \rho \omega_i \mathbf{U}_i \tag{C.36}$$

Flux in terms of mass ratio

$$\mathbf{N}_i = \rho_s \chi_i \mathbf{U}_i \tag{C.37}$$

Fick's law in terms of mass concentration

$$\mathbf{j}_i = -D(\nabla C_i) \tag{C.38}$$

Fick's law in terms of mass fraction

$$\mathbf{j}_i = -\rho D(\nabla \omega_i) \tag{C.39}$$

Fick's law in terms of mass ratio

$$\mathbf{J}_i = -\rho_s D(\nabla \chi_i) \tag{C.40}$$

Cacao Bean

Fick's law in terms of mass ratio

Acetic acid

$$\mathbf{J}_a = -\rho_s D_a (\nabla A_{db}) \qquad \textbf{(C.41)}$$

Moisture

$$\mathbf{J}_w = -\rho_s D_a (\nabla W_{db}) \qquad \textbf{(C.42)}$$

Flux of dry solids

$$\mathbf{N}_s = \rho_s \mathbf{U}_s \qquad \textbf{(C 43)}$$

APPENDIX D
EXPERIMENTAL AND SIMULATION RESULTS

Table D 1. Results of drying test 01

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 1566	1 1566	0 0230	0 0102	0 0161
0.25	0 7758				
0 50	0 6788	0 7009	0 0024	0 0091	0 0124
1 00	0 5419	0.5438	0.0026	0.0077	0.0104
1 50	0 4394	0 4514	0 0033	0 0098	0 0119
2 00	0.3950	0.3879	0.0024	0.0083	0.0141
2.50	0 3305	0.3402	0 0022	0 0087	0 0122
3.00	0.3024	0.3024	0.0026	0.0107	0.0134
3 50	0 2786	0 2714	0 0028	0 0099	0 0155
4.00	0 2580	0 2453	0 0049	0.0109	0 0162
4 50	0 2299	0 2230	0 0023	0 0056	0 0103
5.50	0 1989	0 1666	0 0031	0 0087	0 0131
6 50	0 1731	0 1583	0 0020	0 0058	0 0084
7.50	0 1510	0 1356	0 0018	0 0063	0 0093
8 50	0 1317	0 1172	0 0020	0 0053	0 0089
9.50	0 1146	0 1018	0 0026	0 0082	0 0117
11 50	0 0851	0 0780	0 0027	0 0105	0 0150
12 50		0 0686	0 0011	0 0071	0 0115
13 50	0 0704	0 0618	0 0019	0 0089	0 0149

Air velocity 2.58 m/s
Mean drying air temperature 70 8 °C
Mean ambient temperature 27 0 °C
Mean ambient relative humidity 82 6%

Table D.2. Results of drying test 02

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0.00	1.1035	1.1035	0.0025	0.0106	0.0174
0.17	0.8855	0.9517			
0.25	0.8141				
0.50	0.6920	0.7169	0.0028	0.0113	0.0169
1.00	0.5699	0.5782	0.0035	0.0100	0.0138
1.50	0.4985	0.4954	0.0023	0.0084	0.0132
2.00	0.4478	0.4377	0.0027	0.0071	0.0118
2.50	0.4085	0.3938	0.0028	0.0104	0.0170
3.00	0.3764	0.3586	0.0026	0.0088	0.0134
3.50	0.3493	0.3293	0.0026	0.0083	0.0142
4.00	0.3257	0.3044	0.0013	0.0092	0.0147
4.50	0.3050	0.2829	0.0023	0.0092	0.0138
5.50	0.2696	0.2471	0.0020	0.0096	0.0167
6.50	0.2402	0.2183	0.0026	0.0087	0.0151
7.50	0.2150	0.1946	0.0030	0.0098	0.0151
8.50	0.1930	0.1745	0.0035	0.0088	0.0137
9.50	0.1734	0.1575	0.0022	0.0077	0.0150
11.50	0.1397	0.1303	0.0020	0.0112	0.0147
12.50	0.1250	0.1192	0.0030	0.0110	0.0144
13.50	0.1115	0.1096	0.0026	0.0085	0.0142
14.50	0.0989	0.1007	0.0028	0.0103	0.0134
15.50	0.0871		0.0026	0.0090	0.0147
16.50	0.0812		0.0047	0.0084	0.0146
18.50	0.0760				

Air velocity: 2.55 m/s
Mean drying air temperature: 60.5 °C
Mean ambient temperature: 29.2 °C
Mean ambient relative humidity: 74.1%

Table D.3. Results of drying test 03

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0.00	1.0665	1.0665	0.0039	0.0100	0.0157
0.17	0.9920	0.9702			
0.25	0.9349				
0.50	0.7852	0.7654	0.0026	0.0088	0.0121
1.00	0.6514	0.6175	0.0026	0.0098	0.0135
1.50	0.5643	0.5404	0.0046	0.0099	0.0150
2.00	0.4996	0.4868	0.0043	0.0108	0.0132
2.50	0.4572	0.4459	0.0038	0.0089	0.0136
3.00	0.4225	0.4131	0.0040	0.0083	0.0130
3.50	0.3932	0.3857	0.0037	0.0080	0.0116
4.00	0.3678	0.3622	0.0023	0.0072	0.0114
4.50	0.3454	0.3418	0.0025	0.0063	0.0129
5.50	0.3173	0.3075	0.0035	0.0075	0.0130
6.50	0.2855	0.2794	0.0044	0.0101	0.0134
7.50	0.2583	0.2559	0.0025	0.0083	0.0119
8.50	0.2345	0.2357	0.0031	0.0095	0.0139
9.50	0.2234	0.2182	0.0028	0.0096	0.0120
10.50	0.2044	0.2028	0.0028	0.0079	0.0124
11.50	0.1871	0.1892	0.0035	0.0077	0.0129
12.50	0.1712	0.1770	0.0023	0.0071	0.0112
14.50	0.1430	0.1561	0.0028	0.0073	0.0117
16.50	0.1384	0.1388	0.0024	0.0061	0.0118
18.50	0.1167	0.1246	0.0044	0.0071	0.0149
20.50	0.0972	0.1123	0.0015	0.0076	0.0130
22.50	0.0895	0.1019	0.0033	0.0086	0.0134

Air velocity: 2.58 m/s
Mean drying air temperature: 50.8 °C
Mean ambient temperature: 25.4 °C
Mean ambient relative humidity: 89.7%

Table D 4. Results of drying test 04

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 1768	1 1768	0 0031	0 0091	0 0162
0 17	1 0608	1 1043			
0 25	1 0170				
0 50	0 8607	0 9579	0 0036	0 0102	0 0158
1 00	0 7345	0 7631	0 0025	0 0100	0 0150
1 50	0 6606	0 6468	0 0035	0 0108	0 0164
2 00	0 5882	0 5827	0 0025	0 0108	0 0137
3 00	0 5144	0 5009	0 0033	0 0107	0 0156
4 00	0 4620	0 4476	0 0032	0 0096	0 0140
5 00	0 4073	0 4079	0 0032	0 0113	0 0163
6 00	0 3781	0 3768	0 0031	0 0110	0 0153
7 00	0 3500	0 3510	0 0020	0 0076	0 0127
9 00	0 3143	0 3100	0 0038	0 0095	0 0153
11 00	0 2777	0 2782	0 0022	0 0074	0 0118
13 00	0 2473	0 2469	0 0035	0 0085	0 0124
15 00	0 2312	0 2313	0 0026	0 0076	0 0118
17 00	0 2184	0 2133	0 0043	0 0092	0 0137
19 00	0 1982	0 1972	0 0022	0 0086	0 0121
21 00	0 1799	0 1836	0 0032	0 0086	0 0131
24 00	0 1556	0 1686	0 0025	0 0084	0 0133
27 00	0 1642	0 1531	0 0021	0 0094	0 0125
30 00	0 1450	0 1405	0 0033	0 0077	0 0114
34 00	0 1222	0 1281	0 0032	0 0077	0 0123
38 00	0 1019	0 1171	0 0021	0 0083	0 0125
42 00	0 0837	0 1073			

Air velocity 2.56 m/s
Mean drying air temperature 40 2 °C
Mean ambient temperature 27 7 °C
Mean ambient relative humidity 79 4%

Table D.5 Results of drying test 05

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 1263	1 1263	0 0033	0 0089	0 0211
0 17	0 8554	0 9220			
0.25	0 7855				
0 50	0 6658	0 6846	0 0035	0 0121	0 0217
1 00	0 5462	0 5341	0 0050	0 0108	0 0207
1 50	0 4462	0 4446	0 0027	0 0086	0 0191
2 00	0 3866	0 3827	0 0054	0 0095	0 0195
2.50	0 3381	0 3359	0 0038	0 0090	0 0197
3 00	0 2966	0 2986	0 0055	0 0096	0 0221
3 50	0 2653	0 2680	0 0052	0 0115	0 0211
4 00	0 2410	0 2422	0 0042	0 0094	0 0231
4.50	0 2166	0 2201	0 0043	0 0094	0 0232
5 00	0 1985	0 2008	0 0042	0 0084	0 0202
6 00	0 1670	0 1692	0 0038	0 0102	0 0198
7 00	0 1504	0 1443	0 0037	0 0096	0 0188
8 00	0 1273	0 1240	0 0043	0 0094	0 0227
9 00	0 1070	0 1074	0 0045	0 0103	0 0224
11 00	0 0824	0 0816	0 0018	0 0076	0 0185
12.00	0 0674	0 0717	0 0031	0 0075	0 0178
13 00	0 0636	0 0631	0 0031	0 0089	0 0216

Air velocity 2 58 m/s
Mean drying air temperature 71 2 °C
Mean ambient temperature 29 0 °C
Mean ambient relative humidity 67 9%

Table D 6 Results of drying test 06

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 1584	1 1584	0 0026	0 0083	0 0192
0 17	0 9534	1 0117			
0.25	0 7904				
0 50	0 6825	0 7533	0 0022	0 0087	0 0216
1 00	0 5747	0 5996	0 0030	0 0085	0 0190
1 50	0 4916	0 5107	0 0034	0 0099	0 0185
2 00	0 4368	0 4498	0 0032	0 0121	0 0211
2 50	0 3921	0 4040	0 0028	0 0105	0 0192
3 00	0 3500	0.3676	0 0049	0 0107	0 0201
3 50	0 3298	0.3375	0 0032	0 0113	0 0213
4 00	0 3090	0.3120	0 0036	0 0088	0 0204
4 50	0 2907	0 2900	0 0045	0 0122	0 0215
5.50	0 2594	0 2534	0 0040	0 0101	0 0209
6,50	0 2335	0 2240	0 0029	0 0082	0 0198
7 50	0 2112	0 1996	0 0028	0 0090	0 0202
8 50	0 1917	0 1793	0 0026	0 0080	0 0184
9 50	0 1744	0 1620	0 0038	0 0106	0 0217
11 50	0 1470	0 1342	0 0033	0 0085	0 0216
12.50	0 1360	0 1229	0 0044	0 0093	0 0212
13 50	0 1297	0 1128	0 0034	0 0094	0 0206
14 50	0 1186	0 1038	0 0041	0 0105	0 0213
15 50	0 1083	0 0957	0 0033	0 0083	0 0194
16 50	0 0985	0 0884	0 0043	0 0087	0 0214
18 50	0 0807	0 0722			
20 50	0 0748	0 0609			

Air velocity 2 56 m/s
Mean drying air temperature 60 0 °C
Mean ambient temperature 29 2 °C
Mean ambient relative humidity 72 9%

Table D 7. Results of drying test 07

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 0317	1 0317	0 0034	0 0080	0 0161
0 17	0 9087	0 9244			
0 25	0 8434				
0 50	0 7316	0 7319	0 0041	0 0087	0 0157
1 00	0 6199	0 6119	0 0034	0 0086	0 0173
1 50	0 5546	0 5412	0 0026	0 0067	0 0175
2 00	0 5082	0 4907	0 0032	0 0101	0 0199
2 50	0 4562	0 4518	0 0033	0 0078	0 0155
3 00	0 4268	0 4203	0 0037	0 0082	0 0186
3 50	0 4020	0 3941	0 0035	0 0079	0 0193
4 00	0 3804	0 3713	0 0025	0 0082	0 0202
4 50	0 3615	0 3513	0 0041	0 0087	0 0180
5 50	0 3291	0 3178	0 0037	0 0088	0 0191
6 50	0 3022	0 2901	0 0030	0 0080	0 0152
7 50	0 2791	0 2669	0 0023	0 0072	0 0163
8 50	0 2589	0 2470	0 0029	0 0080	0 0166
9 50	0 2410	0 2298	0 0034	0 0083	0 0164
10 50	0 2249	0 2145	0 0036	0 0079	0 0185
11 50	0 2102	0 2008	0 0023	0 0065	0 0149
12 50	0 1968	0 1883	0 0033	0 0090	0 0174
14 50	0 1728	0 1670	0 0044	0 0086	0 0170
16 50	0 1580	0 1492	0 0027	0 0073	0 0138
18 50	0 1396	0 1344	0 0025	0 0074	0 0142
20 50	0 1330	0 1217	0 0032	0 0091	0 0163
22 50	0 1180	0 1108	0 0025	0 0093	0 0171
24 50	0 1043	0 1024			
26 50	0 0916	0 0887			
28 50	0 0799	0 0789			

Air velocity 2 56 m/s
Mean drying air temperature 49 1 °C
Mean ambient temperature 29 0 °C
Mean ambient relative humidity 68 1%

Table D.8 Results of drying test 08

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 1204	1 1204	0 0030	0 0082	0 0187
0 17	1 0803	1 0589			
0 25	1 0279				
0 50	0 9102	0 9304	0 0031	0 0078	0 0174
1 00	0 7539	0 7498	0 0026	0 0090	0 0189
1 50	0 6500	0 6377	0 0032	0 0087	0 0171
2 00	0 5976	0 5766	0 0028	0 0090	0 0166
2 50	0 5570	0 5321	0 0032	0 0092	0 0205
3 50	0 4957	0 4692	0 0031	0 0086	0 0184
4 50	0 4499	0 4241	0 0034	0 0081	0 0189
5 50	0 4134	0 3896	0 0043	0 0093	0 0199
6 50	0 3829	0 3612	0 0034	0 0088	0 0175
7 50	0 3569	0 3376	0 0048	0 0095	0 0205
9 50	0 3138	0 2993	0 0033	0 0081	0 0162
11 50	0 2790	0 2701	0 0036	0 0105	0 0191
13 50	0 2498	0 2454	0 0028	0 0085	0 0171
15 50	0 2246	0 2246	0 0034	0 0089	0 0184
17 50	0 2025	0 2069	0 0032	0 0088	0 0161
19 50	0 1828	0 1913	0 0025	0 0083	0 0184
21 50	0 1650	0 1781	0 0026	0 0099	0 0171
25 50	0 1640	0 1559	0 0024	0 0081	0 0161
29 50	0 1374	0 1401	0 0032	0 0077	0 0164
33 50	0 1142	0 1262	0 0029	0 0077	0 0155
39 50	0 1042	0 1108	0 0036	0 0088	0 0148
45 50	0 0885	0 0977	0 0025	0 0081	0 0154

Air velocity 2 56 m/s
Mean drying air temperature. 40 2 °C
Mean ambient temperature 28 0 °C
Mean ambient relative humudity 71 4%

Table D 9 Results of drying test 09

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 2386	1 2386	0 0012	0 0091	0 0222
0 25	0 8066				
0 50	0 6807	0 7041	0 0035	0 0089	0 0199
1 00	0 4982	0 5225	0 0012	0 0117	0 0225
1 50	0 4197	0 4196	0 0020	0 0097	0 0219
2 00	0 3640	0 3503	0 0023	0 0109	0 0232
2 50	0 3108	0 2991	0 0023	0 0105	0 0219
3 00	0 2755	0 2592	0 0024	0 0099	0 0204
3 50	0 2457	0 2269	0 0029	0 0092	0 0190
4 00	0 2198	0 2002	0 0023	0 0092	0 0198
4 50	0 1970	0 1777	0 0014	0 0087	0 0166
5 00	0 1766	0 1586	0 0016	0 0093	0 0170
5 50	0 1582	0 1422	0 0027	0 0074	0 0181
6 00	0 1413	0 1279	0 0012	0 0080	0 0164
6 50	0 1258	0 1154	0 0013	0 0069	0 0194
7 00	0 1115	0 1043	0 0020	0 0076	0 0171
7 50	0 0981	0 0945	0 0026	0 0086	0 0190
8 50	0 0839	0 0780	0 0039	0 0094	0 0191
9 50	0 0624	0 0647	0 0016	0 0076	0 0184

Air velocity 2 57 m/s
Mean drying air temperature 79 7 °C
Mean ambient temperature 27 3 °C
Mean ambient relative humidity 77.5%

Table D.10. Results of drying test 10

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0.00	1.0978	1.0978	0.0025	0.0090	0.0208
0.17	0.8543	0.8616			
0.25	0.7343				
0.50	0.6145	0.6448	0.0036	0.0094	0.0179
1.00	0.4747	0.4926	0.0028	0.0094	0.0186
1.50	0.3947	0.4013	0.0030	0.0088	0.0172
2.00	0.3350	0.3377	0.0023	0.0088	0.0157
2.50	0.2814	0.2899	0.0031	0.0100	0.0176
3.00	0.2549	0.2522	0.0037	0.0083	0.0179
3.50	0.2283	0.2214	0.0027	0.0094	0.0163
4.00	0.1952	0.1957	0.0032	0.0098	0.0178
4.50	0.1749	0.1740	0.0020	0.0071	0.0163
5.00	0.1567	0.1556	0.0024	0.0084	0.0153
5.50	0.1402	0.1397	0.0036	0.0081	0.0161
6.00	0.1252	0.1258	0.0020	0.0095	0.0180
6.50	0.1213	0.1136	0.0032	0.0093	0.0182
7.00	0.1085	0.1028	0.0014	0.0087	0.0153
7.50	0.0966	0.0932	0.0030	0.0085	0.0153
8.50	0.0782	0.0770	0.0033	0.0101	0.0158
9.50	0.0658	0.0640	0.0012	0.0078	0.0144
10.50	0.0605		0.0017	0.0072	0.0150

Air velocity: 2.58 m/s
Mean drying air temperature: 79.6 °C
Mean ambient temperature: 28.3 °C
Mean ambient relative humidity: 70.5%

Table D 11. Results of drying test 11

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0.00	1.2904	1.2904	0.0013	0.0108	0.0270
0.25	1.1006				
0.50	0.9489	1.0078	0.0013	0.0108	0.0227
1.00	0.6973	0.7394	0.0014	0.0086	0.0204
1.50	0.5969	0.5979	0.0013	0.0112	0.0198
2.00	0.5257	0.5108	0.0025	0.0109	0.0193
2.50	0.4504	0.4464	0.0025	0.0101	0.0195
3.00	0.4053	0.3958	0.0026	0.0091	0.0194
3.50	0.3671	0.3546	0.0036	0.0110	0.0215
4.00	0.3340	0.3202	0.0035	0.0108	0.0194
4.50	0.3049	0.2907	0.0025	0.0103	0.0201
5.00	0.2788	0.2652	0.0031	0.0096	0.0184
5.50	0.2552	0.2429	0.0026	0.0093	0.0171
6.50	0.2138	0.2057	0.0018	0.0097	0.0168
7.50	0.1784	0.1759	0.0022	0.0083	0.0166
8.50	0.1474	0.1519	0.0036	0.0084	0.0174
9.50	0.1399	0.1317	0.0021	0.0078	0.0167
11.50	0.0926	0.1007	0.0024	0.0075	0.0159
12.50	0.0719	0.0886	0.0011	0.0056	0.0172
13.50	0.0653	0.0781	0.0031	0.0073	0.0162

Air velocity 1.05 m/s
Mean drying air temperature. 70.5 °C
Mean ambient temperature 26.7 °C
Mean ambient relative humidity 73.0%

Table D.12. Results of drying test 12.

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0.00	1.2247	1.2247	0.0012	0.0081	0.0201
0.25	1.1580				
0.50	0.9748	1.0090	0.0026	0.0093	0.0196
1.00	0.7916	0.7903	0.0010	0.0087	0.0179
1.50	0.6445	0.6372	0.0015	0.0091	0.0191
2.00	0.5684	0.5543	0.0019	0.0088	0.0189
2.50	0.5094	0.4936	0.0017	0.0095	0.0186
3.00	0.4613	0.4461	0.0012	0.0097	0.0160
3.50	0.4205	0.4074	0.0018	0.0090	0.0177
4.00	0.3852	0.3747	0.0017	0.0082	0.0191
4.50	0.3541	0.3466	0.0023	0.0074	0.0181
5.50	0.3011	0.3006	0.0037	0.0093	0.0190
6.50	0.2569	0.2641	0.0014	0.0077	0.0165
7.50	0.2191	0.2341	0.0017	0.0075	0.0165
8.50	0.2001	0.2088	0.0018	0.0081	0.0163
9.50	0.1866	0.1875	0.0022	0.0072	0.0143
11.50	0.1461	0.1534	0.0018	0.0082	0.0161
12.50	0.1241	0.1398	0.0019	0.0087	0.0158
13.50	0.1137	0.1277	0.0015	0.0067	0.0132
14.50	0.1049	0.1171	0.0016	0.0073	0.0143
15.50	0.0957	0.1076	0.0011	0.0076	0.0141

Air velocity: 0.97 m/s
Mean drying air temperature: 60.6 °C
Mean ambient temperature: 27.4 °C
Mean ambient relative humidity: 69.2%

Table D.13. Results of drying test 13

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0.00	1.1313	1.1313	0.0007	0.0103	0.0182
0.25	1.0600				
0.50	0.9621	0.9666	0.0010	0.0098	0.0172
1.00	0.7983	0.7983	0.0018	0.0088	0.0194
1.50	0.7024	0.6583	0.0030	0.0091	0.0170
2.00	0.5944	0.5827	0.0027	0.0090	0.0172
2.50	0.5316	0.5287	0.0011	0.0094	0.0171
3.00	0.4785	0.4865	0.0025	0.0080	0.0166
3.50	0.4421	0.4518	0.0014	0.0085	0.0165
4.00	0.4310	0.4226	0.0027	0.0083	0.0153
4.50	0.4027	0.3974	0.0025	0.0080	0.0164
5.00	0.3717	0.3752	0.0021	0.0104	0.0171
5.50	0.3552	0.3556	0.0013	0.0087	0.0148
6.50	0.3257	0.3221	0.0021	0.0076	0.0174
7.50	0.3019	0.2940	0.0026	0.0109	0.0180
8.50	0.2823	0.2702	0.0025	0.0099	0.0186
9.50	0.2660	0.2497	0.0018	0.0106	0.0183
11.50	0.2308	0.2160	0.0026	0.0111	0.0182
12.50	0.2111	0.2017	0.0017	0.0086	0.0152
14.50	0.1860	0.1774	0.0020	0.0091	0.0161
16.50	0.1555	0.1574	0.0015	0.0102	0.0162
18.50	0.1407	0.1407	0.0019	0.0075	0.0142
20.50	0.1241	0.1265	0.0009	0.0088	0.0153
22.50	0.1121	0.1145	0.0017	0.0079	0.0148
24.50	0.0908	0.1041	0.0030	0.0098	0.0159

Air velocity 0.99 m/s
Mean drying air temperature 50.2 °C
Mean ambient temperature 26.8 °C
Mean ambient relative humidity 72.4%

Table D.14. Results of drying test 14

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0.00	1.2440	1.2440	0.0017	0.0077	0.0168
0.25	1.2041				
0.50	1.1126	1.1485	0.0014	0.0105	0.0195
1.00	1.0212	1.0464	0.0013	0.0106	0.0161
1.50	0.9267	0.9452	0.0014	0.0100	0.0169
2.00	0.8217	0.8424	0.0012	0.0085	0.0151
2.50	0.7178	0.7419	0.0011	0.0070	0.0170
3.00	0.6353	0.6496	0.0018	0.0086	0.0152
4.00	0.5483	0.5457	0.0019	0.0091	0.0148
5.00	0.4963	0.4843	0.0014	0.0077	0.0141
6.00	0.4539	0.4392	0.0022	0.0099	0.0162
7.00	0.4180	0.4038	0.0013	0.0084	0.0129
8.00	0.3969	0.3749	0.0013	0.0081	0.0162
10.00	0.3449	0.3292	0.0018	0.0101	0.0154
12.00	0.3124	0.2938	0.0021	0.0074	0.0123
14.00	0.2765	0.2656	0.0016	0.0096	0.0015
16.00	0.2554	0.2420	0.0021	0.0098	0.0140
18.50	0.2316	0.2176	0.0016	0.0071	0.0125
20.50	0.2077	0.2023	0.0031	0.0084	0.0154
22.50	0.1960	0.1886	0.0021	0.0074	0.0131
25.00	0.1715	0.1737	0.0014	0.0086	0.0140
27.00	0.1536	0.1635			
29.00	0.1369	0.1457			
31.00	0.1214	0.1348			
33.00	0.1169	0.1253			
35.00	0.1093	0.1163			
37.00	0.0902	0.1095			

Air velocity 1.02 m/s
Mean drying air temperature 40.4 °C
Mean ambient temperature 27.7 °C
Mean ambient relative humidity 74.4%

Table D 15 Results of drying test 15

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 0986	1 0986	0 0025	0 0097	0 0162
0 50	0 9239	0 9387	0 0032	0 0093	0 0178
1 00	0 7753	0 7761	0 0025	0 0088	0 0146
1 50	0 6383	0 6442	0 0035	0 0087	0 0145
2 00	0 5766	0 5732	0 0036	0 0086	0 0153
2 50	0 5288	0 5217	0 0033	0 0101	0 0158
3 00	0 4896	0 4811	0 0039	0 0924	0 0168
3 50	0 4566	0 4476	0 0036	0 0111	0 0156
4 00	0 4279	0 4193	0 0033	0 0089	0 0137
5 00	0 3801	0 3731	0 0028	0 0094	0 0135
6 00	0 3410	0 3368	0 0037	0 0106	0 0153
7 00	0 3079	0 3066	0 0045	0 0082	0 0163
8 00	0 2793	0 2813	0 0029	0 0098	0 0154
9 00	0 2540	0 2595	0 0036	0 0073	0 0131
10 00	0 2314	0 2407	0 0039	0 0086	0 0151
11 00	0 2110	0 2240	0 0043	0 0094	0 0151
12 00	0 1856	0 2089	0 0027	0 0082	0 0138
14 00	0 1578	0 1836	0 0039	0 0086	0 0146
16 00	0 1451	0 1628	0 0031	0 0101	0 0128
18 00	0 1358	0 1456	0 0022	0 0080	0 0133
20 00	0 1292	0 1310	0 0031	0 0102	0 0138
22 00	0 1123	0 1186	0 0029	0 0086	0 0143
24 00	0 0937	0 1079	0 0031	0 0075	0 0125
26 00	0 0865	0 0988	0 0027	0 0072	0 0126

Air velocity 1 01 m/s
Mean drying air temperature 50 0 °C
Mean ambient temperature 25 8 °C
Mean ambient relative humidity 83 6%

Table D 16 Results of drying test 16

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 1277	1 1277	0 0066	0 0077	0 0250
0 50	1 0010	1 0285	0 0057	0 0064	0 0242
1 00	0 8795	0 9227	0 0061	0 0080	0 0275
1 50	0 7967	0 8204	0 0056	0 0086	0 0230
2 00	0 7018	0 7269	0 0048	0 0071	0 0237
2 50	0 6324	0 6385	0 0066	0 0073	0 0269
3 00	0 5952	0 5800	0 0056	0 0085	0 0253
3 50	0 5404	0 5402	0 0066	0 0084	0 0242
4 50	0 4924	0 4812	0 0059	0 0080	0 0242
5 50	0 4515	0 4373	0 0061	0 0080	0 0232
6 50	0 4174	0 4028	0 0062	0 0087	0 0239
7 50	0 3882	0 3743	0 0069	0 0086	0 0245
8 50	0 3646	0 3503	0 0068	0 0089	0 0268
9 50	0 3449	0 3294	0 0085	0 0090	0 0282
11 50	0 3109	0 2947	0 0075	0 0092	0 0270
13 50	0 2812	0 2663	0 0072	0 0090	0 0259
15 50	0 2515	0 2430	0 0059	0 0080	0 0230
17 50	0 2352	0 2230	0 0047	0 0074	0 0269
19 50	0 2131	0 2055	0 0062	0 0077	0 0272
21 50	0 1932	0 1909	0 0068	0 0081	0 0246
23 50	0 1785	0 1760	0 0075	0 0091	0 0272
25 50	0 1531	0 1677	0 0077	0 0088	0 0265
27 50	0 1520	0 1575	0 0065	0 0089	0 0242
31 50	0 1247	0 1399	0 0063	0 0079	0 0246
37 50	0 1196	0 1208	0 0083	0 0094	0 0245
43 50	0 0893	0 1055	0 0073	0 0085	0 0237

Air velocity 0 97 m/s
Mean drying air temperature 40 0 °C
Mean ambient temperature 25 3 °C
Mean ambient relative humidity 78 0%

Table D.17. Results of drying test 17

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 0877	1 0877	0 0044	0 0115	0 0186
0 50	0 8039	0 8046	0 0026	0 0090	0 0190
1 00	0 6517	0 6221	0 0039	0 0101	0 0150
1 50	0 5326	0 5275	0 0035	0 0113	0 0175
2 00	0 4695	0 4594	0 0060	0 0117	0 0185
2 50	0 4205	0 4066	0 0035	0 0092	0 0148
3 00	0 3804	0 3638	0 0044	0 0089	0 0162
3 50	0 3466	0 3283	0 0028	0 0086	0 0170
4 00	0 3072	0 2981	0 0037	0 0090	0 0184
4 50	0 2854	0 2720	0 0043	0 0113	0 0162
5 00	0 2582	0 2491	0 0049	0 0104	0 0140
6 00	0 2182	0 2111	0 0032	0 0077	0 0172
7 00	0 1944	0 1805	0 0037	0 0101	0 0145
8 00	0 1671	0 1559	0 0041	0 0085	0 0150
9 00	0 1492	0 1355	0 0036	0 0094	0 0150
10 00	0 126	0 1183	0 0043	0 0084	0 0133
11 00	0 1051	0 1046	0 0041	0 0095	0 0164
12 00	0 096	0 0918	0 0025	0 0072	0 0176
13 00	0 0884	0 0810	0 0025	0 0070	0 0152
14 00	0 0721	0 0718	0 0032	0 0084	0 0137
15 00	0 057	0 0638	0 0031	0 0086	0 0142

Air velocity 1.03 m/s
Mean drying air temperature 70 0 °C
Mean ambient temperature 27.2 °C
Mean ambient relative humidity 75 7%

Table D-18. Results of drying test 18

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0.00	1.0513	1.0513	0.0034	0.0083	0.0203
0.50	0.8709	0.8300	0.0037	0.0094	0.0202
1.00	0.6818	0.6487	0.0029	0.0095	0.0173
1.50	0.5887	0.5607	0.0036	0.0096	0.0182
2.00	0.5126	0.4981	0.0021	0.0109	0.0183
2.50	0.4554	0.4496	0.0025	0.0090	0.0184
3.00	0.4195	0.4103	0.0036	0.0093	0.0182
3.50	0.3841	0.3774	0.0030	0.0073	0.0164
4.00	0.3555	0.3492	0.0040	0.0104	0.0183
4.50	0.3264	0.3246	0.0032	0.0095	0.0168
5.00	0.3063	0.3029	0.0040	0.0096	0.0174
6.00	0.2714	0.2664	0.0033	0.0109	0.0182
7.00	0.2450	0.2365	0.0048	0.0106	0.0194
8.00	0.2163	0.2115	0.0039	0.0102	0.0161
9.00	0.1943	0.1902	0.0043	0.0092	0.0158
10.00	0.1731	0.1720	0.0029	0.0093	0.0163
11.00	0.1512	0.1563	0.0017	0.0086	0.0169
12.00	0.1412	0.1426	0.0037	0.0095	0.0172
13.00	0.1229	0.1304	0.0029	0.0096	0.0180
14.00	0.1158	0.1194	0.0035	0.0092	0.0185
15.00	0.1100	0.1098	0.0037	0.0110	0.0173
16.00	0.0952	0.1011	0.0027	0.0105	0.0165
17.00	0.0913	0.0934			
18.00	0.0781	0.0839			

Air velocity= 1.02 m/s
Mean drying air temperature: 60.1 °C
Mean ambient temperature: 27.5 °C
Mean ambient relative humidity: 73.7%

Table D 19 Results of drying test 19

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 0964	1 0964	0 0037	0 0090	0 0205
0 50	0 8397	0 8114	0 0039	0 0080	0 0198
1 00	0 6545	0 6246	0 0058	0 0080	0 0185
1 50	0 5479	0 5287	0 0040	0 0091	0 0170
2 00	0 4731	0 4597	0 0044	0 0089	0 0178
2 50	0 4261	0 4063	0 0049	0 0089	0 0179
3 00	0 3827	0 3633	0 0043	0 0088	0 0184
3 50	0 3459	0 3274	0 0037	0 0072	0 0165
4 00	0 3141	0 2970	0 0039	0 0089	0 0183
4 50	0 2860	0 2706	0 0049	0 0085	0 0207
5 00	0 2609	0 2477	0 0040	0 0100	0 0176
5 50	0 2382	0 2275	0 0054	0 0101	0 0196
6 00	0 2174	0 2095	0 0033	0 0073	0 0174
7 00	0 1837	0 1789	0 0039	0 0085	0 0169
8 00	0 1629	0 1542	0 0037	0 0080	0 0162
9 00	0 1408	0 1339	0 0043	0 0076	0 0154
10 00	0 1157	0 1168	0 0039	0 0079	0 0165
11 00	0 1130	0 1024	0 0048	0 0083	0 0150
12 00	0 1022	0 0900	0 0024	0 0059	0 0172
13 00	0 0831	0 0793	0 0039	0 0076	0 0172
14 00	0 0655	0 0701	0 0048	0 0090	0 0178

Air velocity 1 02 m/s
Mean drying air temperature 70 0 °C
Mean ambient temperature 26 7 °C
Mean ambient relative humidity 73 1%

Table D.20 Results of drying test 20

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 0751	1 0751	0 0034	0 0096	0 0194
0 50	0 9709	0 9720	0 0046	0 0095	0 0184
1 00	0 8336	0 8676	0 0032	0 0079	0 0153
1 50	0 7533	0 7636	0 0048	0 0085	0 0170
2 00	0 6763	0 6714	0 0037	0 0091	0 0151
2 50	0 6071	0 5996	0 0038	0 0096	0 0174
3 00	0 5566	0 5548	0 0039	0 0094	0 0162
3 50	0 5205	0 5203	0 0045	0 0089	0 0159
4 50	0 4707	0 4668	0 0032	0 0084	0 0174
5 50	0 4310	0 4261	0 0046	0 0095	0 0163
6 50	0 3979	0 3937	0 0045	0 0076	0 0177
7 50	0 3595	0 3668	0 0055	0 0098	0 0174
8 50	0 3447	0 3441	0 0036	0 0096	0 0177
9 50	0 3227	0 3243	0 0052	0 0093	0 0169
10 50	0 3069	0 3065	0 0039	0 0093	0 0147
12 50	0 2784	0 2767	0 0043	0 0072	0 0139
14 50	0 2550	0 2518	0 0039	0 0088	0 0138
16 50	0 2374	0 2313	0 0053	0 0101	0 0176
18 50	0 2207	0 2137	0 0030	0 0062	0 0150
20 50	0 2004	0 1979	0 0046	0 0072	0 0133
22 50	0 1819	0 1844	0 0029	0 0063	0 0127
24 50	0 1711	0 1724	0 0041	0 0094	0 0153
26 50	0 1451	0 1629	0 0048	0 0100	0 0158
28 50	0 1367	0 1542	0 0033	0 0084	0 0143
30 50	0 1103	0 1457	0 0023	0 0055	0 0176
34 50	0 1155	0 1308	0 0060	0 0071	0 0147
40 50	0 0858	0 1150	0 0052	0 0075	0 0162

Air velocity 0 97 m/s
Mean drying air temperature 40 0 °C
Mean ambient temperature 25 9 °C
Mean ambient relative humidity 82 3%

Table D.21 Results of drying test 21

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 0825	1 0825	0 0030	0 0066	0 0165
0 50	0 8967	0 8554	0 0029	0 0064	0 0143
1 00	0 6873	0 6538	0 0035	0 0087	0 0150
1 50	0 5782	0 5558	0 0022	0 0053	0 0141
2 00	0 4978	0 4859	0 0030	0 0063	0 0155
2 50	0 4383	0 4314	0 0041	0 0065	0 0133
3 00	0 3987	0 3871	0 0044	0 0066	0 0143
3 50	0 3566	0 3501	0 0035	0 0078	0 0149
4 00	0 3284	0 3184	0 0033	0 0064	0 0129
4 50	0 2996	0 2909	0 0035	0 0073	0 0112
5 00	0 2738	0 2668	0 0029	0 0065	0 0131
6 00	0 2293	0 2265	0 0024	0 0045	0 0141
7 00	0 2016	0 1941	0 0034	0 0066	0 0110
8 00	0 1761	0 1677	0 0033	0 0072	0 0125
9 00	0 1502	0 1459	0 0031	0 0063	0 0115
10 00	0 1344	0 1276	0 0035	0 0067	0 0126
11 00	0 1111	0 1120	0 0023	0 0057	0 0197
12 00	0 0998	0 0988	0 0032	0 0067	0 0117
13 00	0 0903	0 0873	0 0031	0 0061	0 0123
14 00	0 0760	0 0774	0 0028	0 0070	0 0119
15 00	0 0653	0 0687	0 0024	0 0059	0 0107

Air velocity 0 52 m/s
Mean drying air temperature 70 0 °C
Mean ambient temperature 26 6 °C
Mean ambient relative humidity 78 7%

Table D 22. Results of drying test 22.

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 0367	1 0367	0 0022	0 0052	0 0119
0 50	0 9438	0 9045	0 0025	0 0051	0 0120
1 00	0 7925	0 7659	0 0020	0 0067	0 0142
1 50	0 7040	0 6455	0 0032	0 0057	0 0107
2 00	0 6113	0 5753	0 0029	0 0061	0 0127
2 50	0 5526	0 5259	0 0032	0 0059	0 0111
3 00	0 5108	0 4863	0 0028	0 0052	0 0122
3 50	0 4591	0 4534	0 0032	0 0062	0 0130
4 00	0 4265	0 4255	0 0032	0 0055	0 0121
4 50	0 4039	0 4010	0 0023	0 0054	0 0104
5 00	0 3803	0 3795	0 0029	0 0063	0 0123
5 50	0 3555	0 3604	0 0032	0 0075	0 0134
6 50	0 3159	0 3270	0 0030	0 0056	0 0134
7 50	0 2928	0 2990	0 0036	0 0067	0 0118
8 50	0 2701	0 2752	0 0027	0 0048	0 0109
9 50	0 2512	0 2547	0 0029	0 0058	0 0115
10 50	0 2364	0 2367	0 0030	0 0067	0 0106
11 50	0 2195	0 2207	0 0030	0 0059	0 0127
12 50	0 2073	0 2063	0 0018	0 0040	0 0093
14 50	0 1790	0 1815	0 0027	0 0050	0 0102
16 50	0 1570	0 1612	0 0033	0 0073	0 0109
18 50	0 1358	0 1441	0 0031	0 0063	0 0102
20 50	0 1334	0 1297	0 0029	0 0050	0 0095
22 50	0 1131	0 1175	0 0023	0 0050	0 0109
24 50	0 1195	0 1070	0 0037	0 0061	0 0118
26 50	0 1024	0 0983	0 0030	0 0052	0 0101
28 50	0 0865	0 0907			

Air velocity 0 48 m/s
Mean drying air temperature 50 1 °C
Mean ambient temperature 26 4 °C
Mean ambient relative humidity 78 9%

Table D.23 Results of drying test 23

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0.00	1.0912	1.0912	0.0022	0.0069	0.0171
0.50	1.0582	1.0161	0.0028	0.0076	0.0163
1.00	0.9059	0.9370	0.0025	0.0070	0.0161
1.50	0.8168	0.8543	0.0025	0.0070	0.0146
2.00	0.7235	0.7735	0.0028	0.0071	0.0158
2.50	0.6570	0.6954	0.0025	0.0062	0.0171
3.00	0.6026	0.6246	0.0033	0.0070	0.0139
3.50	0.5563	0.5701	0.0025	0.0064	0.0019
4.00	0.5225	0.5334	0.0031	0.0078	0.0122
5.00	0.4850	0.4789	0.0029	0.0080	0.0141
6.00	0.4412	0.4377	0.0026	0.0080	0.0128
7.00	0.4178	0.4058	0.0027	0.0079	0.0116
8.00	0.3948	0.3769	0.0030	0.0065	0.0120
9.00	0.3584	0.3532	0.0027	0.0091	0.0125
11.00	0.3178	0.3146	0.0027	0.0078	0.0113
13.00	0.2834	0.2839	0.0033	0.0082	0.0142
15.00	0.2631	0.2587	0.0023	0.0068	0.0139
17.00	0.2483	0.2375	0.0024	0.0072	0.0123
19.00	0.2258	0.2194	0.0029	0.0083	0.0109
21.00	0.2136	0.2037	0.0031	0.0089	0.0132
23.00	0.1917	0.1904	0.0012	0.0069	0.0127
25.00	0.1784	0.1788	0.0017	0.0069	0.0111
27.00	0.1615	0.1687	0.0028	0.0078	0.0107
31.00	0.1411	0.1507	0.0037	0.0077	0.0114
37.00	0.1122	0.1296	0.0017	0.0059	0.0109
44.00	0.0941	0.1105	0.0028	0.0077	0.0114

Air velocity: 0.47 m/s
Mean drying air temperature: 39.8 °C
Mean ambient temperature: 26.4 °C
Mean ambient relative humidity: 81.9%

Table D.24 Results of drying test 24

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 1409	1 1409	0.0052	0 0064	0 0306
0 50	0 9940	0 9603	0 0050	0 0059	0 0278
1 00	0 8108	0 7722	0 0051	0 0063	0 0258
1 50	0 6469	0 6328	0 0053	0 0060	0 0280
2.00	0 5693	0.5563	0 0053	0 0066	0 0244
2.50	0 4999	0 4992	0 0044	0 0068	0 0236
3 00	0 4594	0 4536	0 0054	0 0075	0 0229
3 50	0 4245	0 4160	0 0048	0 0070	0 0226
4 00	0 3944	0 3841	0 0055	0 0071	0 0242
4 50	0 3680	0 3565	0 0051	0 0076	0 0235
5 00	0 3381	0 3322	0 0065	0 0070	0 0259
5 50	0 3126	0.3107	0 0075	0 0091	0 0270
6 50	0 2782	0.2741	0 0057	0 0066	0 0261
7 50	0 2470	0 2440	0 0054	0 0078	0 0243
8 50	0 2211	0 2184	0 0060	0 0071	0 0240
9 50	0 1981	0 1966	0 0044	0 0064	0 0224
10 50	0 1755	0 1779	0 0052	0 0069	0 0229
11 50	0 1553	0 1617	0 0054	0 0068	0 0223
12.50	0 1333	0 1475	0 0052	0 0067	0 0229
13 50	0 1229	0 1350	0 0051	0 0066	0 0238
14 50	0 1174	0 1238	0 0056	0 0060	0 0244
15 50	0 1124	0 1138	0 0057	0 0071	0 0230
16 50	0 0959	0 1048	0 0065	0 0071	0 0238
17 50	0 0803	0 0968			

Air velocity 0 50 m/s
Mean drying air temperature 60.0 °C
Mean ambient temperature 25 9 °C
Mean ambient relative humidity 75 8%

Table D 25. Results of drying test 25

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0.00	1.1022	1.1022	0.0042	0.0051	0.0229
0.50	0.9413	0.8687	0.0068	0.0065	0.0231
1.00	0.7250	0.6631	0.0048	0.0058	0.0211
1.50	0.5983	0.5629	0.0041	0.0079	0.0209
2.00	0.5038	0.4914	0.0039	0.0059	0.0179
2.50	0.4462	0.4359	0.0049	0.0076	0.0186
3.00	0.3963	0.3907	0.0058	0.0068	0.0215
3.50	0.3619	0.3530	0.0052	0.0077	0.0204
4.00	0.3277	0.3208	0.0047	0.0067	0.0197
4.50	0.2951	0.2930	0.0043	0.0061	0.0176
5.00	0.2779	0.2686	0.0044	0.0060	0.0178
5.50	0.2542	0.2470	0.0047	0.0064	0.0191
6.50	0.2171	0.2105	0.0042	0.0069	0.0176
7.50	0.1761	0.1811	0.0041	0.0060	0.0168
8.50	0.1533	0.1569	0.0037	0.0052	0.0165
9.50	0.1291	0.1367	0.0047	0.0060	0.0180
10.50	0.1245	0.1197	0.0053	0.0059	0.0175
11.50	0.1124	0.1053	0.0039	0.0060	0.0171
12.50	0.0997	0.0928	0.0043	0.0052	0.0162
13.50	0.0772	0.0820	0.0063	0.0073	0.0191
14.50	0.0663	0.0727	0.0039	0.0055	0.0157

Air velocity: 0.55 m/s
Mean drying air temperature: 70.1 °C
Mean ambient temperature: 26.5 °C
Mean ambient relative humidity: 74.7%

Table D.26 Results of drying test 26.

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 3256	1 3256	0 0049	0 0072	0 0210
0 50	1 2703	1 1996	0 0052	0 0077	0 0228
1 00	1 0623	1 0667	0 0061	0 0077	0 0207
1 50	0 9407	0 9324	0 0050	0 0076	0 0203
2 00	0 8144	0 7985	0 0055	0 0075	0 0226
2 50	0 7024	0 6779	0 0049	0 0067	0 0234
3 00	0 5983	0 5951	0 0055	0 0088	0 0222
3 50	0 5537	0 5415	0 0055	0 0066	0 0202
4 00	0 5096	0 4994	0 0053	0 0068	0 0225
4 50	0 4661	0 4645	0 0062	0 0076	0 0220
5 00	0 4345	0 4350	0 0054	0 0066	0 0217
6 00	0 3998	0 3868	0 0054	0 0072	0 0218
7 00	0 3635	0 3489	0 0059	0 0072	0 0216
8 00	0 3235	0 3174	0 0048	0 0071	0 0203
9 00	0 2981	0 2913	0 0058	0 0068	0 0202
10 00	0 2765	0 2683	0 0057	0 0069	0 0219
11 00	0 2579	0 2486	0 0060	0 0078	0 0191
12 00	0 2367	0 2310	0 0053	0 0065	0 0174
14 00	0 2021	0 2013	0 0063	0 0074	0 0201
16 00	0 1755	0 1773	0 0070	0 0068	0 0181
18 00	0 1652	0 1573	0 0043	0 0053	0 0164
20 00	0 1436	0 1408	0 0049	0 0060	0 0175
22 00	0 1250	0 1267	0 0051	0 0067	0 0165
24 00	0 1089	0 1146	0 0049	0 0062	0 0190
26 00	0 0949	0 1049			

Air velocity 0 48 m/s
Mean drying air temperature: 50 2 °C
Mean ambient temperature 25 6 °C
Mean ambient relative humidity 79 3%

Table D.27. Results of drying test 27

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0.00	1.3318	1.3318	0.0066	0.0088	0.0235
0.50	1.2562	1.2563	0.0056	0.0066	0.0203
1.00	1.1943	1.1765	0.0056	0.0071	0.0226
1.50	1.1145	1.0953	0.0064	0.0085	0.0190
2.00	1.0224	1.0119	0.0053	0.0066	0.0215
2.50	0.9210	0.9265	0.0057	0.0065	0.0230
3.00	0.8568	0.8409	0.0066	0.0081	0.0187
3.50	0.7833	0.7584	0.0060	0.0067	0.0207
4.50	0.6267	0.6089	0.0070	0.0088	0.0216
5.50	0.5374	0.5274	0.0066	0.0071	0.0228
6.50	0.4720	0.4738	0.0051	0.0071	0.0215
7.50	0.4293	0.4331	0.0054	0.0074	0.0235
8.50	0.3889	0.4005	0.0060	0.0085	0.0225
9.50	0.3620	0.3732	0.0047	0.0052	0.0196
10.50	0.3367	0.3500	0.0043	0.0057	0.0185
11.50	0.3237	0.3296	0.0067	0.0069	0.0215
13.50	0.2893	0.2954	0.0058	0.0064	0.0185
15.50	0.2570	0.2676	0.0066	0.0082	0.0224
17.50	0.2381	0.2444	0.0049	0.0065	0.0173
19.50	0.2319	0.2250	0.0054	0.0066	0.0168
21.50	0.2112	0.2081	0.0063	0.0061	0.0177
23.50	0.1958	0.1932	0.0052	0.0055	0.0165
25.50	0.1823	0.1809	0.0040	0.0052	0.0148
28.50	0.1569	0.1653	0.0048	0.0048	0.0149
33.50	0.1345	0.1436	0.0055	0.0064	0.0177
38.50	0.1170	0.1270	0.0050	0.0064	0.0145

Air velocity: 0.53 m/s
Mean drying air temperature: 40.1 °C
Mean ambient temperature: 26.6 °C
Mean ambient relative humidity: 77.7%

Table D.28. Results of drying test 28

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 3781	1 3781	0 0047	0 0071	0 0196
0 50	1 2435	1 2035	0 0034	0 0048	0 0131
1 00	1 0261	1 0179	0 0039	0 0071	0 0156
1 50	0 8725	0 8366	0 0039	0 0071	0 0153
2 00	0 7344	0 6789	0 0048	0 0068	0 0147
2 50	0 6144	0 5837	0 0045	0 0055	0 0121
3 00	0 5417	0 5201	0 0044	0 0068	0 0133
3 50	0 4885	0 4704	0 0036	0 0070	0 0148
4 00	0 4427	0 4300	0 0039	0 0069	0 0137
4 50	0 4091	0 3960	0 0033	0 0064	0 0156
5 00	0 3788	0 3668	0 0043	0 0065	0 0128
5 50	0 3585	0 3414	0 0037	0 0059	0 0112
6 00	0 3376	0 3188	0 0046	0 0065	0 0127
7 00	0 2951	0 2804	0 0040	0 0060	0 0121
8 00	0 2609	0 2491	0 0034	0 0064	0 0103
9 00	0 2304	0 2226	0 0026	0 0050	0 0100
10 00	0 2039	0 2002	0 0044	0 0054	0 0103
11 00	0 1838	0 1810	0 0031	0 0052	0 0112
12 00	0 1682	0 1645	0 0038	0 0049	0 0105
13 00	0 1558	0 1499	0 0038	0 0058	0 0117
14 00	0 1299	0 1370	0 0037	0 0055	0 0120
15 00	0 1153	0 1255	0 0035	0 0048	0 0110
16 00	0 1076	0 1155	0 0045	0 0057	0 0126
18 00	0 1000	0 0983			
20 00	0 0864	0 0809			

Air velocity 0 55 m/s
Mean drying air temperature 60 0 °C
Mean ambient temperature 26 4 °C
Mean ambient relative humidity 77 7%

Table D 29 Results of drying test 29

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0.00	1.1368	1.1368	0.0033	0.0055	0.0114
0.50	1.1190	1.0479	0.0032	0.0064	0.0103
1.00	0.9485	0.9505	0.0046	0.0077	0.0127
1.50	0.8488	0.8532	0.0046	0.0068	0.0122
2.00	0.7780	0.7563	0.0048	0.0048	0.0107
2.50	0.6931	0.6656	0.0034	0.0063	0.0089
3.00	0.6310	0.5908	0.0046	0.0059	0.0126
3.50	0.5666	0.5421	0.0030	0.0050	0.0086
4.00	0.5203	0.5041	0.0030	0.0050	0.0094
4.50	0.4844	0.4721	0.0032	0.0043	0.0111
5.00	0.4527	0.4445	0.0037	0.0055	0.0103
5.50	0.4295	0.4200	0.0025	0.0042	0.0098
6.50	0.3881	0.3791	0.0044	0.0059	0.0112
7.50	0.3630	0.3449	0.0035	0.0059	0.0096
8.50	0.3284	0.3162	0.0042	0.0064	0.0125
9.50	0.3060	0.2916	0.0039	0.0054	0.0092
10.50	0.2836	0.2702	0.0025	0.0054	0.0084
11.50	0.2670	0.2514	0.0043	0.0055	0.0093
12.50	0.2473	0.2345	0.0044	0.0064	0.0099
14.50	0.2156	0.2055	0.0026	0.0041	0.0089
16.50	0.1925	0.1817	0.0025	0.0037	0.0106
18.50	0.1665	0.1620	0.0043	0.0050	0.0098
20.50	0.1490	0.1454	0.0040	0.0061	0.0100
22.50	0.1282	0.1312	0.0033	0.0041	0.0108
23.50	0.1238	0.1249	0.0030	0.0050	0.0097
26.00	0.1113	0.1113			
29.00	0.0864	0.0919			
33.00	0.0765	0.0750			

Air velocity 0.09 m/s
Mean drying air temperature 49.9 °C
Mean ambient temperature 24.9 °C
Mean ambient relative humidity 83.2%

Table D.30 Results of drying test 30

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0.00	1.1988	1.1988	0.0053	0.0094	0.0162
0.50	1.1103	1.0451	0.0050	0.0073	0.0144
1.00	0.9069	0.8767	0.0056	0.0099	0.0138
1.50	0.7464	0.7134	0.0031	0.0081	0.0134
2.00	0.6180	0.5959	0.0046	0.0081	0.0135
2.50	0.5367	0.5257	0.0031	0.0078	0.0129
3.00	0.4761	0.4707	0.0035	0.0085	0.0130
3.50	0.4315	0.4254	0.0032	0.0066	0.0130
4.00	0.3901	0.3870	0.0033	0.0074	0.0117
4.50	0.3556	0.3538	0.0026	0.0072	0.0116
5.00	0.3247	0.3248	0.0036	0.0624	0.0129
5.50	0.2983	0.2991	0.0026	0.0086	0.0106
6.50	0.2577	0.2556	0.0037	0.0059	0.0110
7.50	0.2157	0.2201	0.0050	0.0094	0.0118
8.50	0.1955	0.1907	0.0044	0.0084	0.0131
9.50	0.1663	0.1663	0.0044	0.0074	0.0104
10.50	0.1465	0.1456	0.0041	0.0081	0.0109
11.50	0.1322	0.1281	0.0042	0.0079	0.0120
12.50	0.1182	0.1131	0.0043	0.0077	0.0129
13.50	0.1059	0.1000	0.0055	0.0073	0.0117
14.50	0.0938	0.0886	0.0052	0.0083	0.0119
15.50	0.0819	0.0787	0.0041	0.0083	0.0119
16.50	0.0692	0.0700	0.0052	0.0066	0.0122
17.50	0.0661	0.0625			

Air velocity 0.08 m/s
Mean drying air temperature 69.9 °C
Mean ambient temperature 26.3 °C
Mean ambient relative humidity 78.2%

Table D.31. Results of drying test 31

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0.00	1.2552	1.2552	0.0042	0.0062	0.0130
0.50	1.1358	1.1683	0.0035	0.0054	0.0116
1.00	1.0815	1.0742	0.0043	0.0075	0.0116
1.50	0.9798	0.9789	0.0044	0.0061	0.0100
2.00	0.9077	0.8834	0.0033	0.0057	0.0105
2.50	0.8118	0.7889	0.0035	0.0066	0.0101
3.00	0.7406	0.6966	0.0032	0.0060	0.0100
3.50	0.6827	0.6149	0.0036	0.0061	0.0089
4.00	0.5939	0.5572	0.0047	0.0068	0.0103
4.50	0.5204	0.5162	0.0052	0.0058	0.0117
5.00	0.4968	0.4821	0.0040	0.0056	0.0090
5.50	0.4641	0.4528	0.0050	0.0065	0.0097
6.50	0.4012	0.4049	0.0054	0.0061	0.0088
7.50	0.3563	0.3663	0.0049	0.0066	0.0087
8.50	0.3245	0.3341	0.0051	0.0065	0.0106
9.50	0.3017	0.3070	0.0045	0.0074	0.0102
10.50	0.2792	0.2836	0.0031	0.0070	0.0086
11.50	0.2592	0.2631	0.0044	0.0080	0.0119
12.50	0.2430	0.2449	0.0046	0.0085	0.0103
14.50	0.2111	0.2141	0.0039	0.0072	0.0088
16.50	0.1918	0.1889	0.0046	0.0059	0.0098
18.50	0.1614	0.1681	0.0041	0.0059	0.0083
20.50	0.1432	0.1505	0.0039	0.0068	0.0097
22.50	0.1371	0.1356	0.0042	0.0057	0.0092
23.50	0.1349	0.1289	0.0036	0.0070	0.0105
26.00	0.1185	0.1145			
29.00	0.0957	0.0942			
33.00	0.0840	0.0767			

Air velocity 0.11 m/s
Mean drying air temperature 50.1 °C
Mean ambient temperature 25.5 °C
Mean ambient relative humidity 84.1%

Table D.32 Results of drying test 32.

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 3430	1 3430	0 0036	0 0059	0 0149
0 50	1 2507	1 1902	0 0059	0 0093	0 0139
1 00	1 0249	1 0238	0 0062	0 0101	0 0127
1 50	0 8928	0 8560	0 0033	0 0076	0 0146
2 00	0 7493	0 6981	0 0041	0 0075	0 0158
2 50	0 6220	0 5882	0 0048	0 0067	0 0139
3 00	0 5361	0 5198	0 0064	0 0095	0 0120
3 50	0 4725	0 4659	0 0027	0 0065	0 0112
4 00	0 4267	0 4212	0 0063	0 0093	0 0110
4 50	0 3917	0 3833	0 0035	0 0073	0 0135
5 00	0 3595	0 3504	0 0046	0 0074	0 0141
5 50	0 3264	0 3216	0 0060	0 0078	0 0132
6 00	0 3035	0 2961	0 0044	0 0058	0 0117
6 50	0 2805	0 2734	0 0038	0 0066	0 0108
7 50	0 2362	0 2344	0 0034	0 0066	0 0106
8 50	0 2022	0 2024	0 0049	0 0069	0 0116
9 50	0 1714	0 1759	0 0033	0 0068	0 0107
10 50	0 1488	0 1536	0 0037	0 0077	0 0114
11 50	0 1292	0 1348	0 0034	0 0069	0 0115
12 50	0 1084	0 1186	0 0039	0 0051	0 0106
13 50	0 0981	0 1047	0 0050	0 0068	0 0113
14 50	0 0858	0 0926	0 0038	0 0049	0 0092
15.50	0 0787	0 0821	0 0044	0 0072	0 0106
16.50	0 0685	0 0729	0 0046	0 0075	0 0117
17.50	0 0583	0 0649			

Air velocity 0 10 m/s
Mean drying air temperature 70.2 °C
Mean ambient temperature 26 0 °C
Mean ambient relative humidity 79.2%

Table D 33 Results of drying test 33

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0.00	1.3262	1.3262	0.0056	0.0079	0.0162
0.50	1.2815	1.2708	0.0045	0.0083	0.0163
1.00	1.2327	1.2118	0.0044	0.0093	0.0150
1.50	1.1136	1.1520	0.0048	0.0095	0.0156
2.00	0.9944	1.0942	0.0054	0.0076	0.0154
2.50	0.9289	1.0357	0.0032	0.0078	0.0149
3.00	0.8753	0.9758	0.0050	0.0071	0.0137
3.50	0.8300	0.9159	0.0041	0.0074	0.0141
4.00	0.7708	0.8561	0.0048	0.0084	0.0139
4.50	0.7262	0.7938	0.0045	0.0087	0.0128
5.00	0.6653	0.7323	0.0056	0.0077	0.0139
6.00	0.5717	0.6185	0.0060	0.0069	0.0128
7.00	0.5314	0.5337	0.0042	0.0077	0.0099
8.00	0.4872	0.4819	0.0054	0.0093	0.0136
9.00	0.4526	0.4421	0.0054	0.0091	0.0147
10.00	0.4110	0.4094	0.0057	0.0084	0.0139
11.00	0.3867	0.3823	0.0052	0.0087	0.0128
13.00	0.3346	0.3382	0.0049	0.0075	0.0133
15.00	0.3026	0.3033	0.0046	0.0093	0.0157
17.00	0.2754	0.2746	0.0060	0.0089	0.0140
19.00	0.2432	0.2507	0.0033	0.0074	0.0169
21.00	0.2364	0.2302	0.0044	0.0093	0.0184
23.00	0.2186	0.2125	0.0058	0.0095	0.0152
25.00	0.2012	0.1971	0.0047	0.0096	0.0173
27.00	0.1890	0.1845	0.0043	0.0071	0.0174
30.00	0.1748	0.1683	0.0030	0.0098	0.0144
34.00	0.1522	0.1503	0.0036	0.0100	0.0158
40.00	0.1317	0.1291	0.0040	0.0100	0.0145
48.75	0.1169		0.0047	0.0103	0.0157

Air velocity 0.08 m/s
Mean drying air temperature 40.1 °C
Mean ambient temperature 24.3 °C
Mean ambient relative humidity 82.3%

Table D.34. Results of drying test 34

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 3105	1 3105	0 0036	0 0097	0 0269
0 50	1 2040	1 1890	0 0056	0 0080	0 0252
1 00	0 9764	1 0570	0 0048	0 0086	0 0262
1 50	0 8577	0 9221	0 0041	0 0099	0 0239
2 00	0 7435	0 7887	0 0040	0 0071	0 0220
2 50	0 6457	0 6674	0 0053	0 0090	0 0231
3 00	0 5933	0 5821	0 0055	0 0074	0 0201
3 50	0 5388	0 5260	0 0052	0 0088	0 0219
4 00	0 4884	0 4810	0 0054	0 0089	0 0232
4 50	0 4460	0 4432	0 0057	0 0077	0 0232
5 00	0 4152	0 4109	0 0061	0 0091	0 0254
5 50	0 3856	0 3826	0 0059	0 0079	0 0216
6 00	0 3618	0 3576	0 0048	0 0081	0 0219
7 00	0 3185	0 3149	0 0050	0 0087	0 0208
8 00	0 2846	0 2798	0 0049	0 0105	0 0234
9 00	0 2524	0 2501	0 0042	0 0100	0 0228
10 00	0 2281	0 2250	0 0051	0 0085	0 0218
11 00	0 2053	0 2033	0 0047	0 0103	0 0230
12 00	0 1828	0 1845	0 0050	0 0090	0 0209
13 00	0 1679	0 1679	0 0066	0 0110	0 0250
14 00	0 1537	0 1534	0 0057	0 0105	0 0220
15 00	0 1375	0 1405	0 0040	0 0087	0 0213
16 00	0 1243	0 1291	0 0052	0 0093	0 0224
17 00	0 1126	0 1188	0 0055	0 0108	0 0206
23 20	0 0804	0 0742	0 0050	0 0094	0 0219

Air velocity 0 12 m/s
Mean drying air temperature 60 1 °C
Mean ambient temperature 25.2 °C
Mean ambient relative humidity 78 8%

Table D.35 Results of drying test 35

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0 00	1 3106	1 3106	0 0058	0 0107	0 0283
0 50	1.2517	1 1901	0 0048	0 0120	0 0278
1 00	1 0583	1 0589	0 0076	0 0103	0 0263
1 50	0 9251	0 9259	0 0049	0 0097	0 0272
2 00	0 7906	0 7933	0 0069	0 0098	0 0259
2 50	0 7073	0 6719	0 0065	0 0100	0 0274
3 00	0 5975	0 5844	0 0047	0 0087	0 0256
3 50	0 5425	0 5279	0 0059	0 0112	0 0265
4 00	0 4950	0 4826	0 0052	0 0107	0 0233
4 50	0 4543	0 4447	0 0052	0 0105	0 0241
5 00	0 4208	0 4122	0 0043	0 0097	0 0226
5 50	0 3884	0 3838	0 0059	0 0085	0 0235
6 50	0 3435	0 3361	0 0060	0 0103	0 0233
7 50	0 2965	0 2974	0 0052	0 0092	0 0230
8 50	0 2654	0 2652	0 0052	0 0108	0 0216
9 50	0 2388	0 2379	0 0052	0 0093	0 0231
10 50	0 2165	0 2146	0 0062	0 0101	0 0235
11.50	0 1861	0 1943	0 0063	0 0092	0 0220
12.50	0 1707	0 1767	0 0040	0 0079	0 0219
13 50	0 1577	0 1612	0 0053	0 0084	0 0229
14 50	0 1374	0 1475	0 0061	0 0103	0 0225
15 50	0 1237	0 1353	0 0072	0 0118	0 0252
16 50	0 1116	0 1243	0 0064	0 0114	0 0249
17 50	0 1043	0 1145	0 0055	0 0093	0 0232

Air velocity 0 09 m/s
Mean drying air temperature 60 0 °C
Mean ambient temperature 25 4 °C
Mean ambient relative humidity 77 3%

Table D.36. Results of drying test 36

Time (hour)	Dry basis moisture content		Dry basis acid concentrations		
	Measured	Simulated	Citric acid	Lactic acid	Acetic acid
0.00	1.3160	1.3160	0.0058	0.0107	0.0283
0.50	1.2523	1.2591	0.0048	0.0120	0.0278
1.00	1.2172	1.2009	0.0076	0.0103	0.0263
1.50	1.1010	1.1422	0.0049	0.0097	0.0272
2.00	1.0185	1.0840	0.0069	0.0098	0.0259
2.50	0.9545	1.0244	0.0063	0.0100	0.0274
3.00	0.9022	0.9641	0.0047	0.0087	0.0256
3.50	0.8480	0.9014	0.0059	0.0112	0.0265
4.00	0.7820	0.8391	0.0052	0.0107	0.0233
4.50	0.7186	0.7749	0.0052	0.0105	0.0241
5.00	0.6756	0.7133	0.0043	0.0097	0.0226
6.00	0.5803	0.6007	0.0059	0.0085	0.0235
7.00	0.5266	0.5247	0.0060	0.0103	0.0233
8.00	0.4726	0.4753	0.0052	0.0092	0.0230
9.00	0.4392	0.4373	0.0052	0.0108	0.0216
10.00	0.4111	0.4060	0.0052	0.0093	0.0231
12.00	0.3655	0.3564	0.0062	0.0101	0.0235
14.00	0.3310	0.3181	0.0063	0.0092	0.0220
16.00	0.3027	0.2871	0.0040	0.0079	0.0219
18.00	0.2689	0.2616	0.0053	0.0084	0.0229
20.00	0.2487	0.2401	0.0061	0.0103	0.0225
22.00	0.2236	0.2213	0.0072	0.0118	0.0252
24.00	0.2111	0.2049	0.0064	0.0114	0.0249
26.00	0.1988	0.1916	0.0055	0.0093	0.0232
29.00	0.1822	0.1742	0.0046	0.0110	0.0230
33.00	0.1651	0.1548			
39.75	0.1412				
46.80	0.1195	0.1079			

Air velocity 0.11 m/s
Mean drying air temperature 40.0 °C
Mean ambient temperature 25.4 °C
Mean ambient relative humidity 78.3%

APPENDIX E
FORTRAN PROGRAM FOR SIMULATING TRANSPORT PHENOMENA IN THE DRYING OF FULLY EXPOSED CACAO BEANS

The computer program was written in FORTRAN 77 with some implementations of FORTRAN 90 to simulate temperature and mass concentration profiles, as well averages for finite slab geometries. It consists of a main module and four major subroutines which constitutes the core of the program. The main program is basically used for process data input, to call the major subroutines and to output computed results. Three of the subroutines were developed for solving the partial differential equations of the drying model The third subroutine was developed to generate three-dimensional grid for finite slabs. Several auxiliary modules were also included to compute the physical properties of the product, ambient and drying air Four subroutines of the Numerical Recipes Software package (Press et al , 1992) were incorporated in the subroutine written for estimating mass diffusivity These subroutines were used as provided or with the introduction of some minor modifications. Their names are listed at the end of this appendix

```
C*************************************************
      PROGRAM MAIN_DRY_CACAO
C*************************************************
C     PROGRAM FOR SIMULATING DRYING
C     OF FULLY EXPOSED FERMENTED CACAO
C I/O NOMENCLATURE OF VARIABLES
C I/O TD:  DRYING AIR TEMPERATURE (C)
C I/O TA.  AMBIENT AIR TEMPERATURE (C)
C I   TW   AMBIENT WET BULB TEMPERATURE (C)
C I/O RH   AMBIENT REL. HUMIDITY (DECIMAL)
C I/O VA   AIR VELOCITY (M/S)
C I/O T0.  PRODUCT INITIAL TEMPERATURE (C)
C I/O W0   INITIAL MOISTURE (DECIMAL, D.B.)
C I/O C0   INITIAL ACETIC ACID CONC. (DEC.  DB)
C I/O DUR. TIME DURATION OF THE PROCESS (S)
C I/O DT   TIME INCREMENT (S)
C I/O LX.  NO OF SPACE INTERVALS   X DIRECTION
C I/O MY   NO OF SPACE INTERVALS  Y DIRECTION
C I/O NZ.  NO OF SPACE INTERVALS   Z DIRECTION
C I/O PTIME. PRINTING TIME INTERVAL (S)
C I   IPX   PRINTING STEP IN THE X DIRECTION
C I   IPY   PRINTING STEP IN THE Y DIRECTION
C I   KPZ   PRINTING STEP IN THE Z DIRECTION
C O   T     NODE TEMPERATURE (C)
C O   W     NODE MOISTURE (DECIMAL, DB)
C O   C     NODE ACID CONTENT (DECIMAL, DB)
C O   TMA.  PRODUCT AVERAGE TEMPERATURE (C)
C O   WMAR  PRODUCT AVERAGE MOISTURE (DEC.  D.B.)
C O   CMAR. PRODUCT AV. ACIDITY (DEC.  D.B.)
C O   X0    INITIAL BEAN LENGTH (M)   X DIRECTION
C O   Y0    INITIAL BEAN WIDTH (M)   Y DIRECTION
C O   Z0    INITIAL THICKNESS (M)   Z DIRECTION (M)
C O   X.    NODE POSITION IN THE X DIRECTION (M)
C O   Y     NODE POSITION IN THE Y DIRECTION (M)
C O   Z.    NODE POSITION IN THE Z DIRECTION (M)
C O   XMASS  INITIAL BEAN MASS (KG)
C O   RHO0  INITIAL BEAN DENSITY (KG/M3)
C O   TIME   ELAPSED TIME (S)
C     DX     SPACE INCREMENT   X DIRECTION (M)
C     DY     SPACE INCREMENT   Y DIRECTION (M)
C     DZ     SPACE INCREMENT   Z DIRECTION (M)
C     I    INDEX FOR SPACE IN THE X DIRECTION
C     J    INDEX FOR SPACE IN THE Y DIRECTION
C     K    INDEX FOR SPACE IN THE Z DIRECTION
C*************************************************
      COMMON /TEMP/   T(15,15,15),TI(15,15,15)
      COMMON /MOIST/  W(15,15,15),WI(15,15,15)
      COMMON /ACID/   C(15,15,15),CI(15,15,15)
      COMMON /WLOSS/
W1X(15,15),W1Y(15,15),W1Z(15,15)
      COMMON /HEATFG/
HFGX(15,15),HFGY(15,15),HFGZ(15,15)
      COMMON /SPGRID/X(15),Y(15),Z(15), DX(15),
DY(15), DZ(15),AX(15,15),AY(15,15),AZ(13,13),
DV(15,15,15)
      COMMON /OUTPUT/TD,TA,TW,VA,TEMP,C0, X0
Y0,Z0,A0,VOL0,XMASS,RHOI,RHOID,XHI,YA,DT
      COMMON /DIFF/
TK(100),WK(100),V2(100),CT,WE,WO
      COMMON /TAIR/
TDB(100),TWB(100),RHA(100),RHDB(100),YAA(100)
C*************************************************
C     OPEN FILE FOR INPUTING PROCESS DATA
      OPEN(UNIT=1, FILE='DRY.IN')
C     OPEN FILE FOR OUTPUTING RESULTS
      OPEN(UNIT=2,FILE='DRYSS.PRN',ACCESS='APPEND'
STATUS='UNKNOWN')
C     READ PRODUCT INITIAL CONDITIONS AND
PROCESS DATA
C     DRYING AMBIENT AND WET BULB
TEMPERATURES (C),
C     REL. HUMIDITY (DECIMAL) AND AIR
VELOCITY (M/S)
      READ(UNIT=1,FMT='(//,4F10.2)')TD,TA,TWA,VA
C     INITIAL PRODUCT TEMPERATURE, MOISTURE
CONTENT,AND ACETIC ACID CONC.  AND BC'S
READ(UNIT=1,FMT='(/,F10.2,2F10.4)')T0,W0,C0,A0
C     PROCESS DURATION AND TIME INCREMENT
      READ(UNIT=1,FMT='(/,2F10.2)')DUR,DT
C     NO OF SPACE SUBINTERVALS (X, Y & Z AXIS)
      READ(UNIT=1,FMT='(/,3I5)')LX,MY,NZ
C     CONDITIONS FOR PRINTING RESULTS
READ(UNIT=1,FMT='(/,F10.2,3I5)')PTIME,IPX,IPY,KPZ
C     READ PROCESS DISCRETE DATA  TIME (TI)
DRMC (WI)
C     AMBIENT DRY AND WET BULB TEMP
      ICT=0
      DO WHILE(.NOT.EOF(1))
        ICT=ICT+1
READ(UNIT=1,FMT='(4F10.4)')TI(ICT),WI(ICT),
TDB(ICT),TWB(ICT)
        END DO
        CLOSE (UNIT=1)
        WO=W0
C     COMPUTE AVERAGE DRYING CONDITIONS
      CALL MOISTAIR(TA,TWA,RHA,TD,RHDD,YA,A)
C     COMPUTE ACTUAL DRYING CONDITIONS
      DO I= 1 ICT
        CALL
MOISTAIR(TDB(I),TWB(I),RHA(I),TD,RHDD(I),YAA(I))
        END DO
C     COMPUTE PHYSICAL PROPERTIES FOR INITIAL
CONDITIONS
        CALL SIZE(W0,X0,Y0,Z0,A0,VOL0,XMASS,RHOI)
        CALL
AIRPROP(TD,VA,X0,Y0,Z0,A0,RHOA,CPA,XKA,XMUA,
XD,RE,XHI,XJ0,XK,W0)
C     COMPUTE NO OF NODES FOR EACH DIRECTION
        LL= LX+1
        MM=MY+1
        NN=NZ+1
C     SET INITIAL CONDITIONS FOR TEMP  & MOIST
      DO I= 1,LL
        DO J= 1 MM
          DO K= 1 NN
            T(I,J,K)=TE
            TI(I,J,K)=TE
            W(I,J,K)=W0
            WI(I,J,K)=W0
            C(I,J,K)=C0
            CI(I,J,K)=C0
          END DO
        END DO
C     ASSIGN INITIAL VALUES TO MOISTURE &
TEMPERATURE AVERAGES
        TMAR= TE
        WMAR=W0
C     ASSIGN INITIAL VALUES TO HEAT & MASS
TRANSFER COEFFICIENTS
```

```
      XH=XH0
      XKW=XKW0
C     ASSIGN INITIAL VALUES TO CONTROL
VARIABLES
      PTI=0.0
      SHTI=0.0
      TIME=0.0
      WSTOP=0.06
      IPTIME=INT(PTIME)
      ISHTI=300
C     START ITERATIVE PROCEDURE
      DO WHILE (WSTOP.LE.WEAR.AND.TIME.LE.DUR)
C     RESET PRINTING AND SHRINKAGE TIME STEPS
      IF(INT(PTI).EQ.IPTIME) THEN
        PTI=0.0
        ELSE IF(INT(SHTI).EQ.ISHTI) THEN
          SHTI=0.0
        END IF
C     CHECK TIME & MOISTURE FOR SHRINKING
THE DOMAIN
      IF(SHTI.EQ.0.0.AND.WBAR.GE.0.20) THEN
C     COMPUTE NEW VALUES FOR BEAN SIZE
        CALL
SIZE(WBAR,XLL,YMM,ZNN,A,VOL,XM,RO)
        CALL
AIRPROP(TD,VA,XLL,YMM,ZNN,A,RHOA,CPA,
XKA,XMUA,XO,RE,XH,DH,XKW)
C       COMPUTE HALF DIMENSIONS
        XL=XLL/2.0
        YM=YMM/2.0
        ZN=ZNN/2.0
C     GENERATE OR REFRESH SPACE GRID
        CALL GRID3D(XL,YM,ZN,LX,MY,NZ)
        ELSE
        END IF
C     CHECK TIME FOR AVERAGING AND
OUTPUTTING RESULTS
      IF(TIME.EQ.0.0.AND.PTI.EQ.0.0) THEN
C     OUTPUT TEMPERATURE AND MOISTURE
CONTENT AND ACETIC ACID CONCENTRATION
        CALL OUTPUT(TIME,DUR,PTIME,PTI
P,KPY,KPZ,LX,MY,NZ)
        CLOSE(UNIT=2)
      END IF
C     SEARCH FOR ACTUAL MOISTURE FRACTION
        CALL LOCATE(TI,ICT,TIME,JH)
        YA=YAAZ(JH)
      IF(TIME.EQ.0.0.OR.PTI.EQ.0.0) THEN
C     COMPUTE AVERAGES OVER BEAN VOLUME
        CALL
AVERAGE(LL,MM,NN,TIME,DUR,CBAR,WBAR,TBAR)
        ELSE
      END IF
C     COMPUTE MOISTURE PROFILE
        CALL MOIST3D(YA,XK,WTIME,DT,LX,MY,NZ)
C     UPDATE MOISTURE SB TWEEN TWO
CONSECUTIVE TIME STEPS
        DO I=1,LL
          DO J=1,MM
            DO K=1,NN
              W(I,J,K)=W1(I,J,K)
            END DO
          END DO
        END DO
C     COMPUTE TEMPERATURE PROFILE
        CALL TEMP3D(TD,XH,TIME,DT,LX,MY,NZ)
C     UPDATE TEMPERATURES IN TIME
        DO I=1,LL
          DO J=1,MM
            DO K=1,NN
              T(I,J,K)=T1(I,J,K)
            END DO
          END DO
        END DO
C     COMPUTE ACID CONCENTRATION PROFILE
        CALL ACID3D(AC0,TIME,DT,LX,MY,NZ)
C     UPDATE ACETIC ACID CONCENTRATIONS IN
TIME
        DO I=1,LL
          DO J=1,MM
            DO K=1,NN
              C(I,J,K)=C1(I,J,K)
            END DO
          END DO
        END DO
C     INCREMENT TIME
        PTI=PTI+DT
        SHTI=SHTI+DT
        TIME=TIME+DT
      END DO                    !end do while
      STOP
      END
C*****************************************************
      SUBROUTINE OUTPUT
(TIME,DUR,PTIME,PTI,PX,PY,KPZ,LX,MY,NZ)
C*****************************************************
C     NTIME  NUMBER OF TIME STEPS
C     NTI    INDEX FOR TIME
C     PTIME  PRINTING INTERVAL IN TIME (S)
C     PTI    CONTROL FOR PRINTING TIME INTERVAL
C     IPX    PRINTING STEP IN X
C     IPY    PRINTING STEP IN Y
C     IPY    PRINTING STEP IN Z
C     LPI    CONTROL VARIABLE FOR PRINTING IN X
C     LPJ    CONTROL VARIABLE FOR PRINTING IN Y
C     LPK    CONTROL VARIABLE FOR PRINTING IN Z
C     IFLAG  FLAG FOR PRINTING IN X
C     JFLAG  FLAG FOR PRINTING IN Y
C     KFLAG  FLAG FOR PRINTING IN Z
C*****************************************************
      COMMON/OUTPUT/LTA,XWA,YA(10,W(C(
X(0,Y(0,Z(0  A(0,VOLE XMA(0,RHO(0 RH,XH(0,XH(0 VA,DT
      COMMON /TEMP/  T(15 15 15) T1(15 15 15)
      COMMON /MOIST/  W(15 15 15)W1(15 15 15)
      COMMON /ACID/  C(15 15 15),C1(15 15 15)
      COMMON /SPGRID/ X(15),Y(15),Z(15), DX(15)
DY(15),DZ(15),AX(15 15),AY(15 15),AZ(15 15)
DV(15 15 15)
C*****************************************************
      IF(TIME.EQ.0.0)THEN
      WRITE(2,FMT='(A)')
      WRITE(2,FMT='(A)')'*****************************
      WRITE(2,FMT='(A)')
      WRITE(2,FMT='(A)')  DRYING OF FULLY EXPOSED
CACAO BEANS'
        WRITE(2,FMT='(A)')
        WRITE(2,FMT='(A)')'*****************************
      WRITE(2,FMT='(A)')    INITIAL CONDITIONS'
      WRITE(2,FMT='(A,F7.1)')' AMBIENT AIR
TEMPERATURE (C)  TA
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      WRITE(2,FMT='(A,F7.4)')' AIR RELATIVE
HUMIDITY )DEC)   RH
      WRITE(2,FMT='(A,F7.1)')' DRYING AIR
TEMPERATURE (C)   TD
      WRITE(2,FMT='(A,F10.8)')' DRYING AIR REL
HUMIDITY    RHD
      WRITE(2,FMT='(A,F7.2)')' AIR VELOCITY (M/S)
 VA
      WRITE(2 FMT='(A,F7.2)')' HEAT TRANSFER COEF
(W/M2/C)   XH0
      WRITE(2,FMT='(A,F7.1)')' BEAN TEMPERATURE
(C)       TI
      WRITE(2,FMT='(A,F7.4)')' MOISTURE CONTENT
(DB)      W0
      WRITE(2,FMT='(A,F8.4)')' ACETIC ACID CONTENT
(DB)    ,C0
      WRITE(2,*)
      WRITE(2,FMT='(A)')' PRODUCT SHAPE
FINITE SLAB'
      WRITE(2,FMT='(A,F9.4)')' BEAN LENGTH (M)
 ,X0
      WRITE(2,FMT='(A,F9.4)')' BEAN WIDTH (M)
 Y0
      WRITE(2,FMT='(A,F9.4)')' BEAN THICKNESS (M):
 Z0
      WRITE(2,FMT='(A,F10.4)')' BEAN WEIGHT (KG).
 ,XMAS0
      WRITE(2,FMT='(A,F5.4)')' BEAN DENSITY (KG/M3).
 ,RHO0
      WRITE(2 *)
      WRITE(2,FMT='(A,F10.4)')' PROCESS DURATION
(S):    ,DUR
      WRITE(2,*)
      WRITE(2,FMT='(A,F10.6)')' TIME INCREMENT (S)
 ,DT
      WRITE(2 *)
      WRITE(2,FMT='(A,I6)')' NUMBER OF
SUBINTERVALS IN X   ,LX
      WRITE2,FMT='(A,I6)')' NUMBER OF
SUBINTERVALS IN V   ,MY
      WRITE(2,FMT='(A,I6)')' NUMBER OF
SUBINTERVALS IN Z   ,NZ
      WRITE(2 *)
      WRITE(2,FMT='(A,F10.4)')' PRINTING TIME STEP
(S):  ,PTIME
      WRITE(2 *)
      RETURN
      ELSE
        WRITE(UNIT=2,FMT='(A,F17.2)')
     1    ELAPSED TIME (S)  ,TIME
        WRITE(UNIT=2,FMT='(A)')
     1    X       Y       Z       W       A
      END IF
       DO 60 I=1,LX+1
C        START CONTROL FOR PRINTING STEP IN X
         IF(I.EQ.1)THEN
           LPX=0
           IFLAG=0
         ELSE
           LPX=LPX+1
         END IF
         IF(I.EQ.1.OR.LPX.EQ.IPX)THEN
           IFLAG=1
           LPX=0
         ELSE
           END IF
C          END CONTROL FOR PRINTING STEP IN X
C          START CONTROL FOR PRINTING STEP IN Y
           DO 50 J=1,MY+1
C          START CONTROL FOR PRINTING STEP IN Y
           IF(J.EQ.1)THEN
             MPY=0
             JFLAG=0
             ELSE
             MPY=MPY+1
           END IF
           IF(J.EQ.1.OR.MPY.EQ.IPY)THEN
             JFLAG=1
             MPY=0
             ELSE
           END IF
C          END CONTROL FOR PRINTING STEP IN Y
           DO 40 K=1,NZ+1
C          START CONTROL FOR PRINTING STEP IN Z
           IF(K.EQ.1)THEN
             NPZ=0
             KFLAG=1
             ELSE
             NPZ=NPZ+1
           END IF
           IF(K.EQ.1.OR.NPZ.EQ.KPZ)THEN
             KFLAG=1
             NPZ=0
             ELSE
           END IF
C          END CONTROL FOR PRINTING STEP IN Z
           IF(TIME.EQ.0.0.OR.PTI.EQ.I.AND.IFLAG.EQ.1
     1       AND.JFLAG.EQ.1.AND.KFLAG.EQ.1)THEN
             KFLAG=0
             WRITE(UNIT=2,FMT='(3E10.6,F8.2,2F8.4)')
     1       X(I),Y(J),Z(K),T(I,J,K),W1(I,J,K),C1(I,J,K)
           END IF
  40     CONTINUE
         IFLAG=0
  50   CONTINUE
       IFLAG=0
  60 CONTINUE
       RETURN
       END
C*************************************************
      SUBROUTINE MOIST3D
(VA,XKW,TIME,DT,L,M,N)
C*************************************************
C    SUBROUTINE TO CALCULATE MOISTURE
DISTRIBUTION IN TIME AND SPACE DURING
DRYING OF CACAO BEANS
C I/O NOMENCLATURE OF VARIABLES
C I  VA,    MASS FRACTION OF DRYING AIR
C                (KG WATER VAPOR/KG MOIST AIR)
C I  XKW    MASS TRANSFER COEFFICIENT
(KG M2/S)
C I  TIME,  ELAPSED TIME IS)
C I  DT     TIME INCREMENT (S)
C I  L,     NO OF SUBINTERVALS  X DIRECTION
C I  M,     NO OF SUBINTERVALS  V DIRECTION
C I  N,     NO OF SUBINTERVALS =Z DIRECTION
C  O W_   MOISTURE CONTENT (DECIMAL, D. B.)
C    T      NODE TLMPERATURE (C)
C    WL     WATER LOSS AT SURFACE NODE (KG/S)
C    Y5     MASS FRACTION OF AIR AT THE
SURFACE (KG WATER VAPOR/KG MOIST AIR)
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C   DIFF    MOISTURE DIFFUSIVITY (M2/S)
C   RHOD=  DENSITY OF DRY BONE MATERIAL
(KG/M3)
C   AW     WATER ACTIVITY  (DECIMAL)
C   I      INDEX FOR SPACE IN THE X DIRECTION
C   J      INDEX FOR SPACE IN THE Y DIRECTION
C   K      INDEX FOR SPACE IN THE Z DIRECTION
C   LL.    NUMBER OF NODES IN THE X DIRECTION
C   MM     NO OF NODES IN THE Y DIRECTION
C   NN     NUMBER OF NODES IN THE Z DIRECTION
C   DX     SPACE INCREMENT IN THE X DIRECTION
C   DY     SPACE INCREMENT IN THE Y DIRECTION
C   DZ     SPACE INCREMENT IN THE Z DIRECTION
C   X      NODE POSITION IN THE X DIRECTION (M)
C   Y      NODE POSITION IN THE Y DIRECTION (M)
C   Z      NODE POSITION IN THE Z DIRECTION (M)
C   AX     AREA PERP TO THE X DIRECTION (M2)
C   AY     AREA PERP TO THE Y DIRECTION (M2)
C   AZ     AREA PERP TO THE Z DIRECTION (M2)
C   DV     ELEMENT VOLUME (M3)
C**********************************************
      DIMENSION DIFF(15,15,15)
      COMMON /TEMP/   T(15,15,15),TT(15,15,15)
      COMMON /MOISY/  W(15,15,15),W1(15,15,15)
      COMMON /WLOSS/
WLX(15,15),WLY(15,15),WLZ(15,15)
      COMMON /LEAT/GF
HFGX(15,15),HFGY(15,15),HFGZ(15,15)
      COMMON /SPGRID/ X(15),Y(15),Z(15), DX(15),
DY(15),DZ(15),AX(15,15),AY(15,15),AZ(15,15),
DV(15,15,15)
C**********************************************
C   COMPUTE NUMBER OF NODES
      LL=L+1
      MM=M+1
      NN=N+1
C   COMPUTE DENSITY OF DRY BONE MATERIAL
      IF(TIME.EQ.0.0) THEN
        WW=0.0
        CALL
RZN(WW,RX,RY,RZ,A,VOL,XMASS,RHOD)
      ELSE
      ENDIF
C   COMPUTE MOISTURE DIFFUSIVITY OF NODE
(I,J,K) AND AVERAGE
      SS=0.0
      DO I=1,LL
        DO J=1,MM
          DO K=1,NN
            CALL
DIFFUR(TIME,DT,T(I,J,K),W(I,J,K),DIFF(I,J,K))
          END DO
        END DO
      END DO
CCCC
C   CORNER ELEMENT VOLUMES (8)
C   1   CENTER NODE: ORIGIN OF COORDINATE
SYSTEM  (1,1,1)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX1=(DIFF(1,1,1)+DIFF(2,1,1))/2.0
      DIFFWY2=(DIFF(1,1,1)+DIFF(1,2,1))/2.0
      DIFFWZ2=(DIFF(1,1,1)+DIFF(1,1,2))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX2=DIFFWX2*AX(1,1)/DX(1)
      BY2=DIFFWY2*AY(1,1)/DY(1)
      BZ2=DIFFWZ2*AZ(1,1)/DZ(1)
      DIFFCOEF=BX2+BY2+BZ2
C     COMPUTE MOISTURE FLOW DUE TO
DIFFUSION
      WDIFFX=BX2*W(2,1,1)
      WDIFFY=BY2*W(1,2,1)
      WDIFFZ=BZ2*W(1,1,2)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(1,1,1)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(1.0-DIFFCOEF/COEFF)*
W(1,1,1)
      W1(1,1,1)=WMP
C   2   EXTERNAL NODE AT THE END OF X EDGE
(LL,1,1)
C     COMPUTE EQUILIBRIUM MASS FRACTION AT
SURFACE
      CALL HEND_MODIF(T(LL,1,1),AW,W(LL,1,1))
      CALL VAPOR_FRACTION(T(LL,1,1),AW,YS)
C     COMPUTE RATE OF MOISTURE LOSS BY
EVAPORATION
      WLX(1,1)=XKW*AX(1,1)*(YS-YA)
      TOTEVAP=WLX(1,1)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX1=(DIFF(LL-1,1,1)+DIFF(LL,1,1))/2.0
      DIFFWY2=(DIFF(LL,1,1)+DIFF(LL,2,1))/2.0
      DIFFWZ2=(DIFF(LL,1,1)+DIFF(LL,1,2))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX1=DIFFWX1*AX(1,1)/DX(LL)
      BY2=DIFFWY2*AY(LL,1)/DY(1)
      BZ2=DIFFWZ2*AZ(LL,1)/DZ(1)
      DIFFCOEF=BX1+BY2+BZ2
C     COMPUTE MOISTURE FLOW DUE TO
DIFFUSION
      WDIFFX=BX1*W(LL-1,1,1)
      WDIFFY=BY2*W(LL,2,1)
      WDIFFZ=BZ2*W(LL,1,2)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(LL,1,1)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(1.0-DIFFCOEF/COEFF)*
W(LL,1,1)
      W1(LL,1,1)=WMP TOTEVAP/COEFF/RHOD
C   3   EXTERNAL NODE AT THE END OF Y EDGE
(1,MM,1)
C     COMPUTE EQUILIBRIUM MASS FRACTION AT
SURFACE
      CALL HEND_MODIF(T(1,MM,1),AW,W(1,MM,1))
      CALL VAPOR_FRACTION(T(1,MM,1),AW,YS)
C     COMPUTE RATE OF MOISTURE LOSS BY
EVAPORATION
      WLY(1,1)=XKW*AY(1,1)*(YS-YA)
      TOTEVAP=WLY(1,1)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX2=(DIFF(1,MM,1)+DIFF(2,MM,1))/2.0
      DIFFWY1=(DIFF(1,M,1)+DIFF(1,MM,1))/2.0
      DIFFWZ2=(DIFF(1,MM,1)+DIFF(1,MM,2))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX2=DIFFWX2*AX(MM,1)/DX(1)
      BY1=DIFFWY1*AY(1,1)/DY(M)
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      BZ2=DIFFW22*AZ(I,MM)/DZ(I)
      DIFFCOEF=BX2+BY1+BZ2
C     COMPUTL MOISTURE FLOW DUE TO
DIFFUSION
      WDIFFX=BX2*W(2,MM I)
      WDIFFY=BY1*W(I,M1)
      WDIFFZ=BZ2*W(I,MM2)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      CDEFF=DV(I,MM,I)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/CDEFF+(1.0-DIFFCOEF/CDEFF)*
W(I,MM,I)
      W(I,MM,1)=WMP-TOTEVAP/CDEFF/RHOD
C  4  EXTERNAL NODE AT THE END OF Z EDGE
(I,I,NN)
C     COMPUTE EQUILIBRIUM MASS FRACTION AT
SURFACE
      CALL HEND_MODIF(T(I_I,NN),AW,W(I_I,NN))
      CALL VAPOR_FRACTION(T(I_I,NN),AW,YS)
C     COMPUTE RATE OF MOISTURE LOSS BY
EVAPORATION
      WL2(I_I)=XKW*AZ(I_I)*(YS-YA)
      TOTEVAP=WL2(I_I)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX2=(DIFF(I_I,NN)+DIFF(2,I,NN))/2.0
      DIFFWY2=(DIFF(I_I,NN)+DIFF(I,2,NN))/2.0
      DIFFWZ1=(DIFF(I_I,N)+DIFF(I_I,NN))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX2=DIFFWX2*AX(I,NN)/DX(I)
      BY2=DIFFWY2*AY(I,NN)/DY(I)
      BZ1=DIFFWZ1*AZ(I,I)/DZ(N)
      DIFFCOEF=BX2+BY2+BZ1
C     COMPUTE MOISTURE FLOW DUE TO
DIFFUSION
      WDIFFX=BX2*W(2,I,NN)
      WDIFFY=BY2*W(I,2,NN)
      WDIFFZ=BZ1*W(I_I,N)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(I_I,NN)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(1.0-DIFFCOEF/COEFF)*
W(I_I,NN)
      W(I_I,NN)=WMP-TOTEVAP/COEFF/RHOD
C  5  EXTERNAL NODE AT THE Y-Z INTERSECT
(I,MM,NN)
C     COMPUTE EQUILIBRIUM MASS FRACTION AT
SURFACE
      CALL
HEND_MODIF(T(I,MM,NN),AW,W(I,MM NN))
      CALL VAPOR_FRACTION(T(I,MM NN),AW,YS)
C     COMPUTE RATE OF MOISTURE LOSS BY
EVAPORATION
      WL2(I,NN)=XKW*AY(I NN)*(YS-YA)
      WL2(I,MM)=XKW*AZ(I,MM*)(YS-YA)
      TOTEVAP=WL2(I,NN)+WL2(I,MM)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX2=(DIFF(I,MM,NN)+DIFF(2,MM NN))/2.0
      DIFFWY1=(DIFF(I,M NN)+DIFF(I,MM NN))/2.0
      DIFFWZ1=(DIFF(I,MM,N)+DIFF(I,MM,NN))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX2=DIFFWX2*AX(MM,NN)/DX(I)
      BY1=DIFFWY1*AY(I,NN)/DY(M)
      BZ1=DIFFWZ1*AZ(I,MM)/DZ(N)
      DIFFCOEF=BX2+BY1+BZ1
C     COMPUTL MOISTURE FLOW DUE TO
DIFFUSION
      WDIFFX=BX2*W(2,MM,NN)
      WDIFFY=BY1*W(I,MM,NN)
      WDIFFZ=BZ1*W(I,MM,2)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(I,MM,I)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(1.0-DIFFCOEF/COEFF)*
W(I,MM,NN)
      W(I,MM,NN)=WMP-TOTEVAP/COEFF/RHOD
C  6  EXTERNAL NODE AT THE Y-Z
INTERSECTION (LL,MM,1)
C     COMPUTE EQUILIBRIUM MASS FRACTION AT
SURFACE
      CALL
HEND_MODIF(T(LL,MM,1),AW,W(LL,MM 1))
      CALL VAPOR_FRACTION(T(LL,MM,1),AW,YS)
C     COMPUTE RATE OF MOISTURE LOSS BY
EVAPORATION
      WLX(MM,1)=XKW*AX(MM 1)*(YS-YA)
      WLY(LL 1)=XKW*AY(LL,1)*(YS-YA)
      TOTEVAP=WLX(MM 1)+WLY(LL,1)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX1=(DIFF(L,MM 1)+DIFF(LL,MM 1))/2.0
      DIFFWY1=(DIFF(LL,M 1)+DIFF(LL,MM 1))/2.0
      DIFFW22=(DIFF(LL,MM,1)+DIFF(LL,MM,2))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX1=DIFFWX1*AX(MM,1)/DX(L)
      BY1=DIFFWY1*AY(LL,1)/DY(M)
      BZ2=DIFFWZ2*AZ(LL,MM)/DZ(1)
      DIFFCOEF=BX1+BY1+BZ2
C     MOISTURE FLOW DUE TO DIFFUSION
      WDIFFX=BX1*W(LL,MM,1)
      WDIFFY=BY1*W(LL M 1)
      WDIFFZ=BZ2*W(LL,MM,2)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(LL,MM,1)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(1.0-DIFFCOEF/COEFF)*
W(LL,MM,1)
      W(LL,MM,1)=WMP-TOTEVAP/COEFF/RHOD
C  7  EXTERNAL NODE AT THE Z-Y
INTERSECTION (LL,I,NN)
C     COMPUTE EQUILIBRIUM MASS FRACTION AT
SURFACE
      CALL
HEND_MODIF(T(LL,I,NN),AW,W(LL,I NN))
      CALL VAPOR_FRACTION(T(LL,I,NN),AW,YS)
C     COMPUTE RATE OF MOISTURE LOSS BY
EVAPORATION
      WLX(I,NN)=XKW*AX(I NN)*(YS-YA)
      WLZ(LL,I)=XKW*AZ(LL,I)*(YS-YA)
      TOTEVAP=WLX(I NN)+WLZ(LL I)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX1=(DIFF(L,I NN)+DIFF(LL,I NN))/2.0
      DIFFWY2=(DIFF(LL,I NN)+DIFF(LL,I,NN))/2.0
      DIFFWZ1=(DIFF(LL,I,N)+DIFF(LL,I,NN))/2.0
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C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX1=DIFFWX1*AX(I,NN)/DX(I,)
      BY2=DIFFWY2*AY(I,)(I,NN)/DY(I,)
      BZ1=DIFFWZ1*AZ(I,,)(I)Z(IN)
      DIFFCOEF=BX1+BY2+BZ1
C     MOISTURE FLOW DUE TO DIFFUSION
      WDIFFX=(X1*W(I,I,NN)
      WDIFFY=(Y2*W(I,I,2,NN)
      WDIFFZ=9Z  *W(I,I,,N)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(I,I,NN)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(1.0-DIFFCOEF/COEFF)*
W(I,I,NN)
      W(I,I,-I)NN)=WMP TOTEVAP/COEFF/RHOD
C     8--EXTERNAL CORNER OPPOSITE TO THE
CENTER NODE (I,I,MM NN)
C     COMPUTE EQUILIBRIUM MASS FRACTION AT
SURFACE
      CALL
BEND_MODIF(T(I,I,MM,NN),AW W(I,I,MM NN))
      CALL VAPOR_FRACTION(T(I,I,MM,NN),AW,YS)
C     COMPUTE RATE OF MOISTURE LOSS BY
EVAPORATION
      WLX(MM,NN)=XKW*AX(MM,NN)*(YS-YA)
      WLY(I,I,NN)=XKW*AY(I,I,NN)*(YS-YA)
      WLZ(I,I,MM)=XkW*AZ(I,I,MM)*(YS-YA)
      TOTEVAP=WLX(MM NN)+WLY(I,I,NN)+
WLZ(I,I,MM)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX1=(DIFF(I,I,MM,NN)+DIFF(I,I,MM,NN))/2.0
      DIFFWY1=(DIFF(I,I,MNN)+DIFF(I,I,MM,NN))/2.0
      DIFFWZ1=(DIFF(I,I,MM,N)+
DIFF(I,I,MM,NN))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX1=DIFFWX1*AX(MM,NN)/DX(I,)
      BY1=DIFFWY1*AY(I,I,NN)/DY(M)
      BZ1=DIFFWZ1*AZ(I,I,MM)/DZ(N)
      DIFFCOEF=BX1+BY1+BZ1
C     MOISTURE FLOW DUE TO DIFFUSION
      WDIFFX=(X1*W(I,,MM,NN)
      WDIFFY=(Y1*W(I,I,MNN)
      WDIFFZ=(Z1*W(I,I,,MM,N)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(I,I,MM,NN)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(1.0-DIFFCOEF/COEFF)*
W(I,I,MM,NN)
      W(I,I,MM,NN)=WMP- TOTEVAP/COEFF/RHDD
CCCCC
C     NODES ALONG THE SLAB EDGES (12)
      DO I=2,I
C     I   EDGE OF SYMMETRY (INSULATION)   (I, I I)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX1=(DIFF(I,I I,I)+DIFF(I I I))/2.0
      DIFFWX2=(DIFF(I,I I)+DIFFI+I I,I))/2.0
      DIFFWY2=(DIFF(I I)+DIFFI,I2,I))/2.0
      DIFFW22=(DIFF(I,I I)+DIFFI(  2))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX1=DIFFWX1*AX(I  I)/DX(I-I)
      BX2=DIFFWX2*AX(I I)/DX(I)
      BY2=DIFFWY2*AY(I I)/DY(I)
      BZ2=DIFFWZ2*AZ(I,I,DZ(,))
      DIFFCOEI=BX1+BX2+BY2+BZ2
C     MOISTURI FLOW DUE TO DIFFUSION
      WDIFFX=BX1*W(I-I I I)+BX2*W(I+I I I)
      WDIFFY=BY2*W(I,2,I)
      WDIFFZ=BZ2*W(I,I,2)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COLFF=DV(I I )/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF-(1.0-DIFFCOEF/COEFF)*
W(I I I)
      W(I,I I)=WMP
C     2   EXTERNAL EDGE (CONVECTION)
(I,MM NN)
C     COMPUTE EQUILIBRIUM MASS FRACTION AT
SURFACE
      CALL
BEND_MODIF(T(I,MM,NN),AW W(I,MM,NN))
      CALL VAPOR_FRACTION(T(I,MM,NN),AW YS)
C     COMPUTE RATE OF MOISTURE LOSS BY
EVAPORATION
      WLY(I NN)=XKW*AY(I,NN)*(YS-YA)
      WLZ(I MM)=XKW*AZ(I MM)*(YS-YA)
      TOTEVAP=WLY(I,NN)+WLZ(I,MM)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX1=(DIFFI I MM,NN)+DIFF(I,MM,NN))/2.0
      DIFFWX2=(DIFI (I,MM NN)+
DIFF(I+I,MM NN))/2.0
      DIFFWY1=(DIFF(I,M,NN)+DIFF(I,MM NN))/2.0
      DIFFWZ1=(DIFF(I MM,N)+DIFF(I,MM NN))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICILNTS
      BX1=DIFFWX1*AX(MM,NN)/DX(I-I)
      BX2=DIFFWX2*AX(MM NN)/DX(I)
      BY1=DIFFWY1*AY(I,NN)/DY(M)
      BZ1=DIFFWZ1*AZ(I MM)/DZ(N)
      DIFFCOEF=BX1+BX2+BY1+BZ1
C     MOISTURE FLOW DUE TO DIFFUSION
      WDIFFX=BX1*W(I-I MM,NN)+BX2* W(I+1 MM,NN)
      WDIFFY=BY1*W(I,M NN)
      WDIFFZ=BZ1*W(I,MM N)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(I MM NN)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF-(1.0-DIFFCOEF/COEFF)*
W(I,MM,NN)
      W(I,MM,NN)=WMP-TOTFVAP/COEFF/RHDD
C     3   EDGE OF SYMMETRY & CONVECTION
(I,MM-I)
C     COMPUTE EQUILIBRIUM MASS FRACTION AT
SURFACE
      CALL BEND_MODIF(T(I MM-I),AW W(I,MM I))
      CALL VAPOR_FRACTION(T(I,MM,I),AW YS)
C     COMPUTE RATE OF MOISTURE LOSS BY
EVAPORATION
      WLY(I I)=XKW*AY(I,I)*(YS-YA)
      TOTEVAP=WLY(I I)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX1=(DIFFI I MM,I)+DIFF(I MM I))/2.0
      DIFFWX2=(DIFF(I,MM,I)+DIFF(I+I,MM,I))/2.0
      DIFFWY1=(DIFF(I M I)+DIFF(I,MM I))/2.0
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      DIFFWZ2=(DIFF(I,MM,I)+DIFF(IMM,I))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX1=DIFFWX1*AX(MM I)/DX(I-1)
      BX2=DIFFWX2*AX(MM I)/DX(I)
      BY1=DIFFWY1*AY(LI)/DY(M)
      BZ2=DIFFWZ2*AZ(I,MM)/DZ(I)
      DIFFCOEF=BX1+BX2+BY1+BZ2
C     MOISTURE FLOW DIFF TO DIFFUSION
      WDIFFX=5X1 *W(I 1 MM I)+BX2*W(I+ MM.I)
      WDIFFY=-BY1*W(I M I)
      WDIFFZ=-BZ2*W(I MM2)
      TOTDIFF= WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(I,MM I)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(I 0-DIFFCOEF/COEFF)*
W(I MM, I)
      W(I,MM,I)=WMP-TOTEVAP/COEFF/RHOD
C   4  EDGE OF SYMMETRY & CONVECTION
(I I NN)
C     COMPUTE EQUILIBRIUM MASS FRACTION AT
SURFACE
      CALL HEND_MODIF(T(I I NN),AW W(I I,NN))
      CALL VAPOR_FRACTION(T(I I,NN),AW YS)
C     COMPUTE RATE OF MOISTURE LOSS BY
EVAPORATION
      WLX(I)=XKW*AZ(I I)*(YS-YA)
      TOTEVAP=WLX(I I)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX1=(DIFF(I I I NN)+DIFF(I I NN))/2.0
      DIFFWX2=(DIFF(I I NN)+DIFF(I+1 I NN))/2.0
      DIFFWY1=(DIFF(I I NN)+DIFF(I 2 NN))/2.0
      DIFFWZ1=(DIFF(I I N)+DIFF(I I,NN))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX1=DIFFWX1*AX(I,NN)/DX(I I)
      BX2=DIFFWX2*AX(I NN)/DX(I)
      BY2=DIFFWY2*AY(I,NN)/DY(I)
      BZ1=DIFFWZ  *AZ(I I)/DZ(NN)
      DIFFCOEF=BX1+BX2+BY2+BZ1
C     MOISTURE FLOW DIFF TO DIFFUSION
      WDIFFX=8X1 *W(I-1 NN)+BX2*W(I+1 NN)
      WDIFFY= BY2*W(I 2,NN)
      WDIFFZ=-BZ1 *W(I I N)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF= DV(I, I NN)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(I.0-DIFFCOEF/COEFF)*
W(I NN)
      W(I I,NN)=WMP-TOTEVAP/COEFF/RHOD
    END DO       ! *** end mI I in loop ***
CCCCC
    DO I=2,M
C   5  EDGE OF SYMMETRY (INSULATION)  (I,J,I)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX2=(DIFF(I,J I)+DIFF(2,J I))/2.0
      DIFFWY1=(DIFF(I,J I I)+DIFF(I,J I))/2.0
      DIFFWY2=(DIFF(I,J I)+DIFF(I,J+1 I))/2.0
      DIFFWZ2=(DIFF(I,J I)+DIFF(I,J,2)/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX2=DIFFWX2*AX(I )/DX(1)
      BY1=DIFFWY1*AY(I I)/DY(J-I)
      BY2=DIFFWY2*AY(I,I)/DY(J)
      BZ2=DIFFWZ2*AZ(I,J,I)/DZ(I)
      DIFFCOEF=BX2+BY1+BY2+BZ2
C     MOISTURE FLOW DIFF TO DIFFUSION
      WDIFFX=BX2*W(2,J NN)
      WDIFFY=-BY1*W(I,J-1)+BY2*W(I,J+1)
      WDIFFZ=-BZ2*W(I,J,2)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(I,J I)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(I 0-DIFFCOEF/COEFF)*
W(I,J,NN)
      W(I,J,I)=WMP
C   6  EXTERNAL EDGE (CONVECTION)  (I,J,NN)
C     COMPUTE EQUILIBRIUM MASS FRACTION AT
SURFACE
      CALL HEND_MODIF(T(I,J,NN),AW W(I,J,NN))
      CALL VAPOR_FRACTION(T(I,J,NN),AW YS)
C     COMPUTE RATE OF MOISTURE LOSS BY
EVAPORATION
      WLX(J NN)=XKW*AZ(J NN)*(YS-YA)
      WLZ(I,J-)=XKW*AZ(I,J)*(YS-YA)
      TOTEVAP=WLX(I NN)+WLZ(I,J)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX1=(DIFF(I-,J,NN)+DIFF(I,J,NN))/2.0
      DIFFWY1=(DIFF(I,J,I NN)+DIFF(I I, NN))/2.0
      DIFFWY2=(DIFF(I,J,NN)+DIFF(I,J+1,NN))/2.0
      DIFFWZ1=(DIFF(I,J N)+DIFF(I,J,NN))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX1=DIFFWX1*AX(I,NN)/DX(I,)
      BY1=DIFFWY1*AY(I,I NN)/DY(J-I)
      BY2=DIFFWY2*AY(I,NN)/DY(J)
      BZ1=DIFFWZ1*AZ(I,J,I)/DZ(N)
      DIFFCOEF=BX1+BY1+BY2+BZ1
C     MOISTURE FLOW DUE TO DIFFUSION
      WDIFFX=-BX1*W(I,J NN)
      WDIFFY=-BY1*W(I,J I,NN)+BY2*W(I,J+I,NN)
      WDIFFZ=-BZ1*W(I,J,N)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(I,I, NN)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(I 0-DIFFCOEF/COEFF)*
W(I,J,NN)
      W(I,J,NN)=WMP-TOTEVAP/COEFF/RHOD
C   7  EDGE OF SYMMETRY & CONVECTION
(I,J,NN)
C     COMPUTE EQUILIBRIUM MASS FRACTION AT
SURFACE
      CALL HEND_MODIF(T(I,J NN),AW W(I,J,NN))
      CALL VAPOR_FRACTION(T(I,J NN),AW YS)
C     COMPUTE RATE OF MOISTURE LOSS BY
EVAPORATION
      WLZ(I,J)=XKW*AZ(I,J)*(YS-YA)
      TOTEVAP=WLZ(I,J)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX2=(DIFF(I,J,NN)+DIFF(2,J,NN))/2.0
      DIFFWY1=(DIFF(I,J-I,NN)+DIFF(I,J NN)/2.0
      DIFFWY2=(DIFF(I,J,NN)+DIFF(I,J+1 NN))/2.0
      DIFFWZ1=(DIFF(I,J,N)+DIFF(I,J,NN))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX2=DIFFWX2*AX(I,NN)/DX(I)
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      BY1=DIFFWY1*AY(I,NN)/DY(J-1)
      BY2=DIFFWY2*AY(I,NN)/DY(J)
      BZ1=DIFFWZ1*AZ(I,J)/DZ(K)
      DIFFCOEF=BX2+BY1+BY2+BZ1
C     MOISTURE FLOW DUE TO DIFFUSION
      WDIFFX=-BX2*W(I,J,NN)
      WDIFFY=-BY1*W(I,J,NN)+BY2*W(I,J+1,NN)
      WD FFZ=BZ1*W(I,J,N)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(I,J,NN)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(1.0-DIFFCOEF/COEFF)*
W(I,J,NN)
      W1(I,J,NN)=WMP-TOTEVAP/COEFF-RHOD
C     II  EDGE OF SYMMETRY & CONVECTION
(LL,J,1)
C     COMPUTE EQUILIBRIUM MASS FRACTION AT
SURFACE
      CALL HEND_MODIFY(LL,J,1),AW W(LL,J,1))
      CALL VAPOR_FRACTION(T(LL,J,1) AW.YS)
C     COMPUTE RATE OF MOISTURE LOSS BY
EVAPORATION
      WLX(J 1)=-XKW*AX(J 1)*(YS-YA)
      TOTEVAP=WLX(J 1)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX1=(DIFF(LL,J 1)+DIFF(LL,J))/2 II
      DIFFWY1=(DIFF(LL,J 1 1)+DIFF(LL,J ))/2.0
      DIFFWY2=(DIF(0 LL,J1)+DIFF(LL,J+1))/2 II
      DIFFWZ2=(DIFF(LL,J 1)+DIFF(LL,J,2))/2. II
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX1=DIFFWX1*AX(0 1)*DX(L)
      BY1=DIFFWY1*AY(LL,J)/DY(J-1)
      BY2=DIFFWY2*AY(LL,J)/DY(J)
      BZ1=DIFFWZ1*AZ(LL,J)/DZ(1)
      DIFFCOEF=BX1+BY1+BY2+BZ1
C     MOISTURE FLOW DUE TO DIFFUSION
      WDIFFX=0X1*W(LL,J 1)
      WDIFFY=BY1*W(LL,J 1 1)+BY2*W(LL,J+1 1)
      WDIFFZ=-bZ2*W(LL,J,2)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(LL,J 1)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(1.0-DIFFCOEF/COEFF)*
W(LL,J 1)
      W1(LL,J,1)=WMP-TOTFVAP/COEFF/RHOD
    END DO          ! *** end of I do loop ***
CCCCC
    DO K=2,N
C     II  EDGE OF SYMMETRY (INSULATION)   (1 ,K)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX2=(DIFF(1 LK)+DIFF(2 1 K))/2.0
      DIFFWY2=(DIFF(1 1,K)+DIFF(1,2 K))/2.0
      DIFFWZ1=(DIFF(1 1 K-1)+DIFF(1 1 K))/2.0
      DIFFWZ2=(DIF(1 1,K)+DIFF(1 1 K+1))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX2=DIFFWX2*AX(1,K)/DX(1)
      BY2=DIFFWY2*AY(1 K)/DY(1)
      BZ1=DIFFWZ1*AZ(1 1)/DZ(K 1)
      BZ2=DIFFWZ2*AZ(1,1)/DZ(K)
      DIFFCOEF=BX2+BY2+BZ1+BZ2
C     MOISTURE FLOW DUE TO DIFFUSION
      WDIFFX=-BX2*W(2 1,K)
      WDIFFY=-BY2*W(1,2,K)
      WDIFFZ=-bZ1*W(1 1,K-1)+BZ2*W(1,1 K+1)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(1,1,K)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(1 0-DIFFCOEF/COEFF)*
W(1 1 K)
      W1(1 1 K)=WMP
C     I3   EXTERNAL EDGE (CONVECTION)
(LL,MM,K)
C     COMPUTE EQUILIBRIUM MASS FRACTION AT
SURFACE
      CALL
HEND_MODIFY(LL,MM,K),AW W(LL,MM,K))
      CALL VAPOR_FRACTION(T(LL,MM,k) AW YS)
C     COMPUTE RATE OF MOISTURE LOSS BY
EVAPORATION
      WLX(MM,K)=-XKW*AX(MM,K)*(YS-YA)
      WLY(LL,K)=-XKW*AY(LL K)*(YS YA)
      TOTEVAP=WLX(MM,K)+WLY(LL,K)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX1=(DIFF(I MM K)+DIFF(LMM K))/2 II
      DIFFWY1=(DIFF(LL,MM,K)+DIFF(LL,MM,K))/2.0
      DIFFWZ1=(DIFF(LL,MM,K 1)+
DIFF(LL,MM,k-1))/2.0
      DIFFWZ2=(DIFF(LL,MM,K)+
DIFF(LL MM K+1))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX1=DIFFWX1*AX(MM K)/DX(L)
      BY1=DIFFWY1*AY(LL,K)/DY(M)
      BZ1=DIFFWZ1*AZ(LL,MM)/DZ(K 1)
      BZ2=DIFFWZ2*AZ(LL,MM)/DZ(K)
      DIFFCOEF=BX1+BY1+BZ1+BZ2
C     MOIS TURE FLOW DUE TO DIFFUSION
      WDIFFX=-BX1*W(LMM,K)
      WDIFFY=-BY1*W(LL,M K)
      WDIFFZ=-BZ1*W(LL,MM,K 1)+BZ2*W(LL,MM,K+1)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(LL,MM,K)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(1.0-DIFFCOEF/COEFF)*
W(LL,MM,K)
      W1(LL,MM,K)=WMP-TOTEVAP/COEFF/RHOD
C     II   EDGE OF SYMMETRY & CONVECTION
(I,MM,K)
C     COMPUTE EQUILIBRIUM MASS FRACTION AT
SURFACE
      CALL HEND_MODIFY(I,MM,K),AW W(I,MM,K))
      CALL YAPOR_FRACTION(T(I,MM K),AW YS)
C     COMPUTE RATE OF MOISTURE LOSS BY
EVAPORATION
      WLY(I K)=XKW*AY(I,K)*(YS-YA)
      TOTEVAP=WLY(I K)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX2=(DIFF(1 MM K)+DIFF(2,MM,K))/2.0
      DIFFWY1=(DIFF(I MM,K)+DIFF(I,MM K))/2.0
      DIFFWZ1=(DIFF(I MM,K 1)+DIFF(I,MM,K))/2.0
      DIFFWZ2=(DIFF(I MM K)+DIFF(I,MM,K+1))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX2=DIFFWX2*AX(MM,K)/DX(I)
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      BY1=DIFFWY1*AY(I,K)/DY(M)
      BZ1=DIFFWZ1*AZ(I,M)/DZ(K-1)
      BZ2=DIFFWZ2*AZ(I,M)/DZ(K)
      DIFFCOEF=BX2+EY1+BZ1+BZ2
L     MOISTURE FLOW DUE TO DIFFUSION
      WDIFFX=BX2*W(2,MM,K)
      WDIFFY=-BY1*W(I,M,K)
      WDIFFZ=BZ1*W(I,MM,K-1)+BZ2*W(I,MM,K+1)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(I MM,K)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(1.0-DIFFCOEF/COEFF)*
W(I MM,K)
      W1(I,MM,K)=WMP-TOTEVAP/COEFF/RHOD
C     J2---EDGE OF SYMMETRY & CONVECTION
(L,I,K)
C     COMPUTE EQUILIBRIUM MASS FRACTION AT
SURFACE
      CALL HEND_MODIF(T(L,I,K),AW W(L,I,K))
      CALL VAPOR_FRACTION(T(L,I K) AW YS)
C     COMPUTE RATE OF MOISTURE LOSS BY
EVAPORATION
      WLX(I K)=XKW*AX(I K)*(YS-YA)
      TOTEVAP=WLX(I,K)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX1=(DIFF(L,I,K)+DIFF(L-1,I,K))/2.0
      DIFFWY2=(DIFF(L,I L,K)+DIFF(I I-2,K))/2.0
      DIFFWZ1=(DIF F(L I,K-1)+DIFF(L,I,K))/2.0
      DIFFWZ2=(DIFF(L,I,K)+DIFF(L,I,K+1))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX1=DIFFWX1*AX(I,K)/DX(L)
      BY2=DIFFWY2*AY(L,I,K)/DY(I)
      BZ1=DIFFWZ1*AZ(L,I,)/DZ(K-1)
      BZ2=DIFFWZ2*AZ(L,I,)/DZ(K)
      DIFFCOEF=BX1+EY2+BZ1+BZ2
C     MOISTURE FLOW DUE TO DIFFUSION
      WDIFFX=BX1*W(L I,K)
      WDIFFY=BY2*W(L,I,K)
      WDIFFZ=BZ1*W(L,I,K-1)+BZ2*W(L I,K+1)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(I,L, I K)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(1.0-DIFFCOEF/COEFF)*
W(L,I I,K)
      W1(LL,I,K)=WMP-TOTEVAP/COEFF/RHOD
    END DO        ! *** end nEK do loop ***
CCCCC
C   SLAB SURFACES (6)
    DO I=2,I.
    DO J=3,M
C   I-PLANE OF SYMMCTRY XY  (I,J 1)
C   COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX2=(DIFF(I L,J-1)+DIFF(I,J,I))/2.0
      DIFFWX2=(DIFF(I,J I)+DIFF(I+1,J I))/2.0
      DIFFWY1=(DIFF(I,J-1 1)+DIFF(I,I J))/2.0
      DIFFWY2=(DIFF(I,J I)+DIFF(I,J+1 I))/2.0
      DIFFWZ=(DIFF(I,J I)+DIFF(I,J,I J))/2.0
C   COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX1=DIFFWX1*AX(I I)/DX(I-1)
      BX2=DIFFWX2*AX(I I)/DX(I)
      BY1=DIFFWY1*AY(L,I)/DY(J 1)
      BY2=DIFFWY2*AY(L I)/DY(J)
      BZ=DIFFWZ*AZ(L,I)/DZ(I I)
      DIFFCOEF=BX1+BX2+BY1+BY2+BZ
C     MOISTURE FLOW DUE TO DIFFUSION
      WDIFFX=BX1*W(I-1,J NN)+BX2*W(I+1,J NN)
      WDIFFY=BY1*W(I,J-1,NN)+BY2*W(I,J+1,NN)
      WDIFFZ=BZ1*W(I,J N)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(I,J,NN)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(1.0-DIFFCOEF/COEFF)*
W(I,J,NN)
      W1(I,J,NN)=WMP
C   2  EXTERNAL SURFACE XY   (I,J NN)
C   COMPUTE EQUILIBRIUM MASS FRACTION AT
SURFACE
      CALL HEND_MODIF(T(I,J,NN),AW W(I,J,NN))
      CALL VAPOR_FRACTION(T(I,J,NN),AW YS)
C     COMPUTE RATE OF MOISTURE LOSS BY
EVAPORATION
      WLZ(I,J)=XKW*AZ(I,J)*(YS-YA)
      TOTEVAP=WLZ(I,J)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX1=(DIFF(I I,J,NN)+DIFF(I,J,NN))/2.0
      DIFFWX2=(DIFF(I,J NN)+DIFF(I+1,J NN))/2.0
      DIFFWY1=(DIFF(I,J-1 NN)+DIFF(I,J,NN))/2.0
      DIFFWY2=(DIFF(I,J NN)+DIFF(I,J+1,NN))/2.0
      DIFFWZ1=(DIFF(I,J,N)+DIFF(I,J NN))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX1=DIFFWX1*AX(I,NN)/DX(I-1)
      BX2=DIFFWX2*AX(I,NN)/DX(I)
      BY1=DIFFWY1*AY(I,NN)/DY(J 1)
      BY2=DIFFWY2*AY(I,NN)/DY(J)
      BZ1=DIFFWZ1*AZ(I,J)/DZ(N)
      DIFFCOEF=BX1+BX2+BY1+BY2+BZ1
C     MOISTURE FLOW DUE TO DIFFUSION
      WDIFFX=BX1*W(I-1,J NN)+BX2*W(I+1,J,NN)
      WDIFFY=BY1*W(I,J-1,NN)+BY2*W(I,J+1,NN)
      WDIFFZ=BZ1*W(I,J N)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(I,J,NN)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(1.0-DIFFCOEF/COEFF)*
W(I,J,NN)
      W1(I,J NN)=WMP-TOTEVAP/COEFF/RHOD
    END DO
    END DO        ! *** end of I-J do loops ***
CCCCC
    DO J=1,M
    DO K=2,N
C   J-PLANE OF SYMMETRY YZ  (I,J,K)
C   COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX2=(DIFF(I,J,K)+DIFF(I,J,K))/2.0
      DIFFWY1=(DIFF(I,J I,K)+DIFF(I,J,K))/2.0
      DIFFWY2=(DIFF(I,J,K)+DIF F(I,J+1,K))/2.0
      DIFFWZ1=(DIFF(I,J,K-1)+DIFF(I,J,K))/2.0
      DIFFWZ2=(DIFF(I,J,K)+DIFF(I,J,K+1))/2.0
C   COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX2=DIFFWX2*AX(J,K)/DX(I)
      BY1=DIFFWY1*AY(I,K)/DY(J 1)
      BY2=DIFFWY2*AY(I,K)/DY(J)
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      BZ1=DIFFWZ1*AZ(I,J)/DZ(K-1)
      BZ2=DIFFWZ2*AZ(I,J)/DZ(K)
      DIFFCOEF=BX2+BY1+BY2+BZ1+BZ2
C     MOISTURE FLOW DUE TO DIFFUSION
      WDIFFX=BX2*W(I,J,K)
      WDIFFY=BY1*W(I,J-1,K)+BY2*W(I,J+1,K)
      WDIFFZ=BZ1*W(I,J,K-1)+BZ2*W(I,J,K+1)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFI=DY(I,J,K)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(1.-DIFFCOEF/COEFF)*
W(I,J,K)
      W1(I,J,K)=WMP
C     4 -EXTERNAL SURFACE YZ  (I,J,K)
C     COMPUTE EQUILIBRIUM MASS FRACTION AT
SURFACE
      CALL HEND_MODIF(I,LL,J,K),AW,W(I,J,K))
      CALL YAPOL_FRACTION(T(I,J,K),AW,YS)
C     COMPUTE RATE OF MOISTURE LOSS BY
EVAPORATION
      WLX(I,K)=XKW*AX(I,K)*(YS-YA)
      TOTEVAP=WLX(I,K)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX1=(DIF(I,J,K)+DIF(I-1,J,K))/2.0
      DIFFWY1=(DIF(I,J-1,K)+DIF(I,J,K))/2.0
      DIFFWY2=(DIF(I,J+1,K)+DIF(I,J,K))/2.0
      DIFFWZ1=(DIF(I,J,K-1)+DIF(I,J,K))/2.0
      DIFFWZ2=(DIF(I,J,K)+DIF(I,J,K+1))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX1=DIFFWX1*AX(I,K)/DX(I-1)
      BY1=DIFFWY1*AY(I,J-1)/DY(J-1)
      BY2=DIFFWY2*AY(I,J,K)/DY(J)
      BZ1=DIFFWZ1*AZ(I,J)/DZ(K-1)
      BZ2=DIFFWZ2*AZ(I,J)/DZ(K)
      DIFFCOEF=BX1+BY1+BY2+BZ1+BZ2
C     MOISTURE FLOW DUE TO DIFFUSION
      WDIFFX=BX1*W(I-1,J,K)
      WDIFFY=BY1*W(I,J-1,K)+BY2*W(I,J+1,K)
      WDIFFZ=BZ1*W(I,J,K-1)+BZ2*W(I,J,K+1)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFI=DY(I,J,K)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(1.-DIFFCOEF/COEFF)*
W(I,J,K)
      W1(I,J,K)=WMP-TOTEVAP/COEFF/RHOD
      END DO
    END DO          ! *** end of J-K do loops ***
CCCCC
      DO I=2,L
      DO K=2,N
C     5-PLANE OF SYMMETRY XZ  (I,1,K)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX1=(DIF(I-1,1,K)+DIF(I,1,K))/2.0
      DIFFWX2=(DIF(I,1,K)+DIF(I+1,1,K))/2.0
      DIFFWY2=(DIF(I,1,K)+DIF(I,2,K))/2.0
      DIFFWZ1=(DIF(I,1,K-1)+DIF(I,1,K))/2.0
      DIFFWZ2=(DIF(I,1,K)+DIF(I,1,K+1))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX1=DIFFWX1*AX(I,K)/DX(I-1)
      BX2=DIFFWX2*AX(I,K)/DX(I)
      BY2=DIFFWY2*AY(I,K)/DY(1)
      BZ1=DIFFWZ1*AZ(I,J)/DZ(K-1)
      BZ2=DIFFWZ2*AZ(I,J)/DZ(K)
      DIFFCOEF=BX1+BX2+BY2+BZ1+BZ2
C     MOISTURE FLOW DUE TO DIFFUSION
      WDIFFX=BX1*W(I-1,1,K)+BX2*W(I+1,1,K)
      WDIFFY=BY2*W(I,2,K)
      WDIFFZ=BZ1*W(I,1,K-1)+BZ2*W(I,1,K+1)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFI=DY(I,1,K)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(1.-DIFFCOEF/COEFF)*
W(I,1,K)
      W1(I,1,K)=WMP
C     6 -EXTERNAL SURFACE XZ  (I,MM,K)
C     COMPUTE AVERAGE DIFFUSIVITY
      CALL HEND_MODIF(I,MM,K),AW,W(I,MM,K))
      CALL YAPOL_FRACTION(I,MM,K),AW,YS)
C     COMPUTE RATE OF MOISTURE LOSS BY
EVAPORATION
      WLY(I,K)=XK*AY(I,K)*(YS-YA)
      TOTEVAP=WLY(I,K)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX1=(DIF(I-1,MM,K)+DIF(I,MM,K))/2.0
      DIFFWX2=(DIF(I,MM,K)+DIF(I+1,MM,K))/2.0
      DIFFWY1=(DIF(I,MM,K)+DIF(I,MM,K))/2.0
      DIFFWZ1=(DIF(I,MM,K-1)+DIF(I,MM,K))/2.0
      DIFFWZ2=(DIF(I,MM,K)+DIF(I,MM,K+1))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX1=DIFFWX1*AX(MM,K)/DX(I-1)
      BX2=DIFFWX2*AX(MM,K)/DX(I)
      BY1=DIFFWY1*AY(I,K)/DY(M)
      BZ1=DIFFWZ1*AZ(I,MM)/DZ(K-1)
      BZ2=DIFFWZ2*AZ(I,MM)/DZ(K)
      DIFFCOEF=BX1+BX2+BY1+BZ1+BZ2
C     MOISTURE FLOW DUE TO DIFFUSION
      WDIFFX=BX1*W(I-1,MM,K)+BX2*W(I+1,MM,K)
      WDIFFY=BY1*W(I,M,K)
      WDIFFZ=BZ1*W(I,MM,K-1)+BZ2*W(I,MM,K+1)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFI=DY(I,MM,K)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/COEFF+(1.0-DIFFCOEF/COEFF)*
W(I,MM,K)
      W1(I,MM,K)=WMP-TOTEVAP/COEFF/RHOD
      END DO
    END DO          ! *** end of I-K do loops ***
CCCCC
C     INTERIOR ELEMENT NODES
C     1.  ELEMENT VOLUME XYZ  (I,J,K)
      DO I=2,L
      DO J=2,M
      DO K=2,N
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFWX1=(DIF(I-1,J,K)+DIFF(I,J,K))/2.0
      DIFFWX2=(DIF(I,J,K)+DIFF(I+1,J,K))/2.0
      DIFFWY1=(DIF(I,J-1,K)+DIFF(I,J,K))/2.0
      DIFFWY2=(DIF(I,J,K)+DIFF(I,J+1,K))/2.0
      DIFFWZ1=(DIF(I,J,K-1)+DIFF(I,J,K))/2.0
      DIFFWZ2=(DIF(I,J,K)+DIFF(I,J,K+1))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX1=DIFFWX1*AX(MM,K)/DX(I-1)
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      BX2=DIFFWX2*AX(I,J,K)/DX(I)
      BY1=DIFFWY1*AY(I,K)/DY(J-1)
      BY2=DIFFWY2*AY(I,K)/DY(J)
      BZ1=DIFFWZ1*AZ(I,J)/DZ(K-1)
      BZ2=DIFFWZ2*AZ(I,J)/DZ(K)
      DIFFCOEF=BX1+BX2+BY1+BY2+BZ1+BZ2
C     MOISTURE FLOW DUE TO DIFFUSION
      WDIFFX=BX1*W(I-1,J,K)+BX2*W(I+1,J,K)
      WDIFFY=BY1*W(I,J-1,K)+BY2*W(I,J+1,K)
      WDIFFZ=BZ1*W(I,J,K-1)+BZ2*W(I,J,K+1)
      TOTDIFF=WDIFFX+WDIFFY+WDIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEF9=DV(I,J,K)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
      WMP=TOTDIFF/(COEF9+(1.0-DIFFCOEF/COEF9)*
W(I,J,K)
      W(I,J,K)=WMP
      END DO
     END DO
     END DO        ! *** end of I-J-K do loops ***
     RETURN
     END
C*************************************************
     SUBROUTINE TEMPJN(TA,XH,TIME,DT,L,MAN)
C*************************************************
C    SUBROUTINE TO COMPUTE TEMP DISTRIB
C    IN TIME AND SPACE DURING CACAO DRYING C
     NOMENCLATURE OF VARIABLES
C    TA    DRYING AIR TEMPERATURE (C)
C    XH    CONVEC HT TRANSFER COEFF (W/M2.C)
C    TIME  ELAPSED TIME (S)
C    DT    TIME INCREMENT (S)
C    I     SPACE INDEX IN THE X DIRECTION
C    J     SPACE INDEX IN THE Y DIRECTION
C    K     SPACE INDEX IN THE Z DIRECTION
C    L     NO OF SPACE INTERVALS - X DIRECTION
C    M     NO OF SPACE INTERVALS - Y DIRECTION
C    N     NO OF SPACE INTERVALS  Z DIRECTION
C    T     NODE TEMPERATURE (C)
C    W     NODE MOISTURE CONTENT (DEC  DB)
C    WL    FLOW OF EVAPORATED MOISTURE
(KG/KG/S)
C    HFG   FLOW OF LATENT HEAT OF
VAPORIZATION (W)
C    CP    SPECIFIC HEAT CAPACITY (J/KG C)
C    XKT   THERMAL CONDUCTIVITY (W/M.C)
C    RHO   DENSITY OF THE MATERIAL (KG/M3)
C*************************************************
     DIMENSION
XKT(15,15,15),CP(15,15,15),RHO(15,15,15)
     DIMENSION DELTA(15,15,15)
     COMMON /TEMP/  T(15,15,15),T0(15,15,15)
     COMMON /MOIST/  W(15,15,15),W1(15,15,15)
     COMMON /WLOSS/
WL(15,15,15),WLY(15,15),WLZ(15,15,15)
     COMMON /HEATFG/
HFGX(15,15),HFGY(15,15),HFGZ(15,15)
     COMMON /SPGRID/ X(15),Y(15),Z(15),DX(15),
DY(15),DZ(15),AX(15,15),AY(15,15),AZ(15,15),
DV(15,15,15)
C*************************************************
C    INDICES FOR EXTERNAL NODES
     LL=L+1
     MM=M+1
     NN=N+1

C    SET CHANGE IN TEMPERATURE TO 0.0
     IF(TIME.EQ.0.0) THEN
      DO I=1,LL
       DO J=1,MM
        DO K=1,NN
         DELTA(I,J,K)=0.0
        END DO
       END DO
      END DO
     END IF
C    COMPUTE PHYSICAL PROPERTIES
     DO I=1,LL
      DO J=1,MM
       DO K=1,NN
        TEMPT=T(I,J,K)+DELTA(I,J,K)/2.0
        CALL SIZE(W(I,J,K),XH,Y(I,2),A,V,XM,RHO(I,J,K))
        CALL THERMAL(TEMPT,W(I,J,K),CP(I,J,K),XK)
       END DO
      END DO
     END DO
C    COMPUTE THERMAL CONDUCT OF NODE (I,J,K)
     DO I=1,LL
      DO J=1,MM
       DO K=1,NN
        CALL THERMAL(T(I,J,K),W(I,J,K),C0,XKT(I,J,K))
       END DO
      END DO
     END DO
CCCCC
C    INTERNAL NODES
C    I   CENTER NODE  ORIGIN OF COORD. SYSTEM
(1,1,1)
C    COMPUTE AVERAGE CONDUCTIVITY
     XKTX2=(XKT(I+1,J,K)+XKT(I+1,J,K))/2.0
     XKTY2=(XKT(I,J+1,K)+XKT(I,J,K))/2.0
     XKTZ2=(XKT(I,J,K+1)+XKT(I,J,K))/2.0
C    COMPUTE CONDUCTION RELATED
COEFFICIENTS
     BX2=XKTX2*AX(I,J)/DX(I)
     BY2=XKTY2*AY(I,J)/DY(J)
     BZ2=XKTZ2*AZ(I,J)/DZ(I)
     CONDCOEF=BX2+BY2+BZ2
C    ENERGY FLOW DUE TO CONDUCTION
     CONDX=BX2*T(I+1,J,K)
     CONDY=BY2*T(I,J+1,K)
     CONDZ=BZ2*T(I,J,K+1)
     TOTCOND=CONDX+CONDY+CONDZ
C    COMPUTE TRANSIENT COEFFICIENT
     COEFF=RHO(I,J,K)*CP(I,J,K)*DV(I,J,K)/DT
C    COMPUTE NEW NODE TEMPERATURE
     TMP=TOTCOND/COEFF+(1.0-CONDCOEF/COEFF)*
T(I,J,K)
      T(I,J,K)=TMP
      DELTA(I,J,K)=T(I,J,K)-T0(I,J,K)
C    NODES ALONG THE SLAB EDGES (12)
     DO I=2,L
C    I=EDGE OF SYMMETRY (INSULATION)  (L+1)
C    COMPUTE AVERAGE CONDUCTIVITY
     XKTX1=(XKT(I-1,J,K)+XKT(I,J,K))/2.0
     XKTX2=(XKT(I,J,K)+XKT(I+1,J,K))/2.0
     XKTY2=(XKT(I,J+1,K)+XKT(I,J,K))/2.0
     XKTZ2=(XKT(I,J,K+1)+XKT(I,J,K))/2.0
C    COMPUTE CONDUCTION RELATED
COEFFICIENTS
     BX1=XKTX1*AX(I-1,J)/DX(I-1)
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      BX2=XKTX2*AX(I,J)*DX(I)
      BY2=XKTY2*AY(I,J)*DY(J)
      BZ2=XKTZ2*AZ(I,J)*DZ(I)
      CONDCOEF=BX1+BX2+BY2+BZ2
C     ENERGY FLOW DUE TO CONDUCTION
      CONDX=-BX1*T(I-1,J)+BX2*T(I+1,J)
      CONDY=-BY1*T(I,J-1)+BY2*T(I,J+1)
      CONDZ=-BZ1*T(I,J,K-1)+BZ2*T(I,J,K+1)
      TOTCOND=CONDX+CONDY+CONDZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=RHO(I,J,K)*CP(I,J,K)*DV(I,J,K)/DT
C     COMPUTE NEW NODE TEMPERATURE
      TMP=TOTCOND/COEFF+(1.0-CONDCOEF/COEFF)*
     T(I,J,K)
      T(I,J,K)=TMP
      DELTA(I,J,K)=T(I,J,K)-T(I,J,K)
    END DO          ! *** end of K do loop ***
  END DO            ! *** end of J do loop ***
END DO              ! *** end of I do loop ***
DO K=2,N
C   6- EDGE OF SYMMETRY (INSULATION)  (I,J,K)
C   COMPUTE AVERAGE CONDUCTIVITY
    XKTX2=(XKT(I+1,J,K)+XKT(I,J,K))/2.0
    XKTY2=(XKT(I,J+1,K)+XKT(I,J,K))/2.0
    XKTZ1=(XKT(I,J,K)+XKT(I,J,K-1))/2.0
    XKTZ2=(XKT(I,J,K)+XKT(I,J,K+1))/2.0
C   COMPUTE CONDUCTION RELATED
COEFFICIENTS
    BX2=XKTX2*AX(I,J)*DX(I)
    BY2=XKTY2*AY(I,J)*DY(J)
    BZ1=XKTZ1*AZ(I,J)*DZ(K)
    BZ2=XKTZ2*AZ(I,J)*DZ(K)
    CONDCOEF=BX2+BY2+BZ1+BZ2
C   ENERGY FLOW DUE TO CONDUCTION
    CONDX=BX2*T(I,J,K)
    CONDY=BY2*T(I,J,K)
    CONDZ=BZ1*T(I,J,K-1)-BZ2*T(I,J,K+1)
    TOTCOND=CONDX+CONDY+CONDZ
C   COMPUTE TRANSIENT COEFFICIENT
    COEFF=RHO(I,J,K)*CP(I,J,K)*DV(I,J,K)/DT
C   COMPUTE NEW NODE TEMPERATURE
    TMP=TOTCOND/COEFF+(1.0-CONDCOEF/COEFF)*
   T(I,J,K)
    T(I,J,K)=TMP
    DELTA(I,J,K)=T(I,J,K)-T(I,J,K)
  END DO            ! *** end of K do loop ***
END DO              ! *** end of J do loop ***
END DO              ! *** end of I do loop ***
C   SLAB SURFACES (6)
  DO I=2,L
    DO J=2,M
C   1- PLANE OF SYMMETRY XY  (I,J,1)
C   COMPUTE AVERAGE CONDUCTIVITY
    XKTX1=(XKT(I-1,J,1)+XKT(I,J,1))/2.0
    XKTX2=(XKT(I,J,1)+XKT(I+1,J,1))/2.0
    XKTY1=(XKT(I,J-1,1)+XKT(I,J,1))/2.0
    XKTY2=(XKT(I,J,1)+XKT(I,J+1,1))/2.0
    XKTZ2=(XKT(I,J,1)+XKT(I,J,2))/2.0
C   COMPUTE CONDUCTION RELATED
COEFFICIENTS
    BX1=XKTX1*AX(I,J)*DX(I-1)
    BX2=XKTX2*AX(I,J)*DX(I)
    BY1=XKTY1*AY(I,J)*DY(J-1)
    BY2=XKTY2*AY(I,J)*DY(J)
    BZ2=XKTZ2*AZ(I,J)*DZ(1)
    CONDCOEF=BX1+BX2+BY1+BY2+BZ2
C   ENERGY FLOW DUE TO CONDUCTION
    CONDX=BX1*T(I-1,J,1)+BX2*T(I+1,J,1)
    CONDY=BY1*T(I,J-1,1)+BY2*T(I,J+1,1)
    CONDZ=BZ2*T(I,J,2)
    TOTCOND=CONDX+CONDY+CONDZ
C   COMPUTE TRANSIENT COEFFICIENT
    COEFF=RHO(I,J,1)*CP(I,J,1)*DV(I,J,1)/DT
C   COMPUTE NEW NODE TEMPERATURE
   TMP=TOTCOND/COEFF+(1.0-CONDCOEF/COEFF)*
   T(I,J,1)
    T(I,J,1)=TMP
    DELTA(I,J,1)=T(I,J,1)-T(I,J,1)
    END DO
  END DO            ! *** end of J do loops ***
  DO J=2,M
    DO K=2,N
C   3- PLANE OF SYMMETRY YZ-  (1,J,K)
C   COMPUTE AVERAGE CONDUCTIVITY
    XKTX2=(XKT(1,J,K)+XKT(2,J,K))/2.0
    XKTY1=(XKT(1,J-1,K)+XKT(1,J,K))/2.0
    XKTY2=(XKT(1,J,K)+XKT(1,J+1,K))/2.0
    XKTZ1=(XKT(1,J,K-1)+XKT(1,J,K))/2.0
    XKTZ2=(XKT(1,J,K)+XKT(1,J,K+1))/2.0
C   COMPUTE CONDUCTION RELATED
COEFFICIENTS
    BX2=XKTX2*AX(1,J,K)*DX(1)
    BY1=XKTY1*AY(1,J,K)*DY(J-1)
    BY2=XKTY2*AY(1,J,K)*DY(J)
    BZ1= XKTZ1*AZ(1,J,K)*DZ(K-1)
    BZ2=XKTZ2*AZ(1,J,K)*DZ(K)
    CONDCOEF=BX2+BY1+BY2+BZ1+BZ2
C   ENERGY FLOW DUE TO CONDUCTION
    CONDX=BX2*T(2,J,K)
    CONDY=BY1*T(1,J,K)+BY2*T(1,J+1,K)
    CONDZ=BZ1*T(1,J,K-1)+BZ2*T(1,J,K+1)
    TOTCOND=CONDX+CONDY+CONDZ
C   COMPUTE TRANSIENT COEFFICIENT
    COEFF=RHO(1,J,K)*CP(1,J,K)*DV(1,J,K)/DT
C   COMPUTE NEW NODE TEMPERATURE
   TMP=TOTCOND/COEFF+(1.0-CONDCOEF/COEFF)*
   T(1,J,K)
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```
      T1(I,J,K)=TMP
      DELTA(I,J,K)=T1(I,J,K)-T(I,J,K)
      END DO
    END DO          ! *** end of I-K do loops ***
    DO I=2,L
      DO k=2,N
C     5   PLANE OF SYMMETRY XZ   (I, J, K)
C     COMPUTE AVERAGE CONDUCTIVITY
      XKTX1=(XKT[I-1 I K)+XKT(I I K))/2.0
      XKTX2=(XKT(I,I,K)+XKT(I+1,I,K))/2.0
      XKTY2=(XKT(I,I,K)+XKT(I,2,K))/2.0
      XKTZ1=(XKT(I,I,K-1)+XKT(I,I,k))/2.0
      XKTZ2=(XKT(I,I,K)+XKT(I,I,K+1))/2.0
C     COMPUTE CONDUCTION RELATED
COEFFICIENTS
      BX1=XKTX1*AX(I,K)/DX(I-1)
      BX2=XkTX2*AX(I,K)/DX(I)
      BY2=XkTY2*AY(I,K)/DY(I)
      BZ1=XKTZ1*AZ(I,I)/DZ(K-1)
      BZ2=XKTZ2*AZ(I,I)/DZ(K)
      CONDCOEF=B(X1+BX2+BY2+BZ1+BZ2
C     ENERGY FLOW DUE TO CONDUCTION
      CONDX=-BX1*T(I-1,I,K)+BX2*T(I+1,I,K)
      CONDY=-BY2*T(I,2,K)
      CONDZ=-BZ1*T(I,I,K-1)+BZ2*T(I,I,K+1)
      TOTCOND=CONDX+CONDY+CONDZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFI=RHO(I,I,k)*CP(I,I,k)*DV(I,I,k)/DT
C     COMPUTI. NEW NODE TEMPERATURE
      TMP=TOTCOND/COEFF+(1.0-CONDCOEF/COEFF)*
T(I I K)
        T1(I,I,K)=TMP
        DELTA(I,I,K)=T1(I,I,K)-T(I,I,K)
      END DO
    END DO          ! *** end of I-K do loops ***
C   INTERIOR ELEMENT NODES
C   ELEMENT VOLUME XYZ   (I, J, K)
    DO I=2,L
      DO J=2,M
        DO K=2,N
C     COMPUTE AVERAGE CONDUCTIVITY
      XkTX1=(XKT(I-I,J,k)+XKT(I,J,K))/2.0
      XKTX2=(XKT(I,I,K)+XKT(I+1,I,K))/2.0
      XKTY1=(XKT(I,I I,K)+XKT(I,J,K))/2.0
      XKTY2=(XKT(I,J+k)+XkT(I,I+1,K))/2.0
      XkTZ1=(XkT(I,I I K-I)+XkT(I,I,K))/2.0
      XkTZ2=(XkT(I,I,k)+XkT(I,I,K+1))/2.0
C     COMPUTE CONDUCTION KELATED
COEFFICIENTS
      BX1=XKTX1*AX(I,K)/DX(I-1)
      BX2=XkTX2*AX(I,K)/DX(I)
      BY1=XkTY1*AY(I,k)/DY(J-1)
      BY2=XkTY2*AY(I,K)/DY(I)
      BZ1=XkTZ1*AZ(I,J)/DZ(K-1)
      BZ2=XKTZ2*AZ(I,J)/DZ(K)
      CONDCOEF=BX1+BX2+BY1+BY2+BZ1+BZ2
C     ENERGY FLOW DUE TO CONDUCTION
      CONDX=-BX1*T(I-1,J,K)+BX2*T(I+1,J,K)
      CONDY=-BY1*T(I,J-1,K)+BY2*T(I,J+1,K)
      CONDZ=-BZ1*T(I,J,K-1)+BZ2*T(I,J,K+1)
      TOTCOND=CONDX+CONDY+CONDZ
C     COMPUTE TRANSIENT COFFICIENT
      COEFF=RHO(I,J,K)*CP(I,J,K)*DV(I,J,K)/DT
C     COMPUTE NEW NODE TEMPERATURE
      TMP=TOTCOND/COEFF+(1.0-CONDCOEF/COEFF)*
T(I,J,K)
        T1(I,J,K)=TMP
        DELTA(I,J,K)=T1(I,J,K)-T(I,J,K)
      END DO
    END DO          ! *** end of I-J-K do loops ***
CCCCC
C   SURFACE NODES (NON-CAPACITANCE NODES)
C   NODE TEMPERATURES (T1) = F(T1 INTERIOR
NODES & AIR)
C   2   EXTERNAL NODE AT THE END OF X EDGE
(L, I, I)
C     COMPUTE LATENT HEAT OF VAPORIZATION
      CALL XLHEAT(T(L, I I),W(L, I, I),AW,XL)
C     ENERGY FLOW DUE TO MOISTURE
VAPORIZATION
      HFGX(I I)=WLX(I I)*XL
      TOTHFG=HFGX(I I)
C     COMPUTE AVERAGE CONDUCTIVITY
      XkTX1=(XKT(L,I I)+XKT(L,L,1))/2.0
      XkTY2=(XKT(L,I I)+XKT(L,2,1))/2.0
      Xk/TZ=(XKT(L,I I)+XkT(L,I I,2))/2.0
C     COMPUTE CONDUCTION & CONVECTION
COEFFICIENTS
      BX1=XkTX1*AX(I I)/DX(L)
      AHX=XH*AX(I I)
      BY2=XkTY2*AY(L,I)/DY(I)
      BZ2=YkTZ2*A2(L,L)/DZ(1)
      TOTCOEF=-BX1+BY2+BZ2+AHX
C     ENERGY FLOW DUE TO CONDUCTION
      CONDX=BX1*T(L,I I)
      CONDY=BY2*T(LL,2,I)
      CONDZ=BZ2*T(LL,I,2)
      TOTCOND=CONDX+CONDY+CONDZ
C     ENERGY FLOW DUE TO CONVECTION
      TOTCONV=AHX*TA
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=RHO(L,I I)*CP(L,I I)*DV(L,I I)/DT
C     COMPUTE NEW NODE TEMPERATURE
      TMP=TOTCOND/COEFF+(1.0-TOJCOF/ICOEFF)*
T(L,I I)
        T1(L,I I)=TMP+(TOTCONV TOTHFG)/COEFF
        DFLTA(L,I I)=T1(L,I I)-T(L,I I)
C   3   EXTERNAL NODE AT THE END OF Y EDGE
(I MM,I)
C     COMPUTE LATENT HEAT OF VAPORIZATION
      CALL XI HEAT(T(I MM I),W(I MM I),AW,XL)
C     ENERGY FLOW DUE TO MOISTURE
VAPORIZATION
      HFGY(I I)=WLY(I I)*XL
      TOTHFG=HFGY(I I)
C     COMPUTE AVERAGE CONDUCTIVITY
      XKTX2=(XK(T(I,MM,I)+XKT(2,MM,I))/2.0
      XKTY1=(XKT(I M I)+Xk/T(I MM I))/2.0
      XKTZ2=(Xk/T(I,MM,I)+XkT(I MM,I))/2.0
C     COMPUTE CONDUCTION & CONVECTION
COEFFICIENTS
      BX2=XKTX2*AXIMM I)/DX(I)
      BY1=XkTY1*AYII I)/DYM)
      AHY=XH*AY(I I)
      BZ2=XkTZ2*AZ[I,MM)/DZ(1)
      TOTCOLL=BX2+BY1+BZ2+AHY
C     ENERGY FLOW DUE TO CONDUCTION
      CONDX=-BX2*T(2,MM I)
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      CONDY=HY1*T(1,M 1)
      CONDZ=HZ1* T(1,MM,2)
      TOTCOND=CONDX+CONDY+CONDZ
C     ENERGY FLOW DHE TO CONVECTION
      TOTCONV=AHY*TA
C     COMPUTE TRANSIENT COEFFICIENT
COEFF=RHO(1 MM,1)*CP(1 MM,1)*DV(1,MM,1)/DT
C     COMPUTE NEW NODE TEMPERATURE
      TMP=TOTCOND/COEFF+(1.0-TOTCOEF/COEFF)*
T(1 MM,1)
      T(1),MM 1)=TMP+(TOTCONV TOTHFG)/COEFF
      DELTA(1,MM 1)=T(1 MM,1)-T(1,MM,1)
C     4  EXTERNAL NODE AT THE END OF Z EDGE
(1 1,NN)
C     COMPUTE LATENT HEAT OF VAPORIZATION
      CALL XLHEAT(T(1 1 NN) W(1 1 NN),AW XL)
C     ENERGY FLOW DUE TO MOISTURE
VAPORIZATION
      HFGZ(1,1)=WLZ(1 1)*XL
      TOTHFG=HFGZ(1 1)
C     COMPUTE AVERAGE CONDUCTIVITY
      XKTX2=(XKT(1 1 NN)+XKT(2,1,NN))/2.0
      XKTY2=(XKT(1 1 NN)+XKT(1,2 HH))/2.0
      XKTZ1=(XKT(1 1 N)+XKT(1 1,NN))/2.0
C     COMPUTE CONDUCTION & CONVECTION
COEFFICIENTS
      BX2=XKTX2*AX(1 NN)*DX(1)
      BY2=XKTY2*AY(1 NN)*DY(1)
      BZ1=XKTZ1*AZ(1,1)*DZ(N)
      AHZ=XH*AZ(1 1)
      TOTCOEF=BX2+BY2+BZ1+AHZ
C     ENERGY FLOW DUE TO CONDUCTION
      CONDX=BX2*T(2,1 NN)
      CONDY=BY2*T(1,2 NN)
      CONDZ=BZ1*T(1 1,N)
      TOTCOND=CONDX+CONDY+CONDZ
C     ENERGY FLOW DUE TO CONVECTION
      TOTCONV=AHZ*TA
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=RHO(1,1,NN)*CP(1 1 NN)*DV(1 1,NN)/DT
C     COMPUTE NEW NODE TEMPERATURE
      TMP=TOTCOND/COEFF+(1.0-TOTCOEF/COEFF)*
T(1 1 NN)
      T(1)  1 NN)=TMP+(TOTCONV TOTHFG)/COEFF
      DELTA(1 1 NN)=T(1 1 NN)-T(1 1,NN)
C     5  EXTERNAL NODE AT THE Y-Z INTERSECT
(1,MM,NN)
C     COMPUTE LATENT HEAT OF VAPORIZATION
      CALL
XLHEAT(T(1,MM,NN) W(1,MM NN),AW XL)
C     ENERGY FLOW DUE TO MOISTURE
VAPORIZATION
      HFGY(1 NN)=WLY(1,NN)*XL
      HFGZ(1,MM)=WLZ(1,MM)*XL
      TOTHFG=HFGY(1 NN)+HFGZ(1 MM)
C     COMPUTE AVERAGE CONDUCTIVITY
      XKTX2=(XKT(1 MM NN)+XKT(2 MM,NN))/2.0
      XKTY1=(XKT(1 M NN)+XKT(1 MM NN))/2.0
      XKTZ=(XKT(1,MM,NN)+XKT(1,MM,NN))/2.0
C     COMPUTE CONDUCTION & CONVECTION
COEFFICIENTS
      BX2=XKTX2*AX(MM,NN)*DX(1)
      BY1=XKTY1*AY(1 NN)*DY(M)
      AHY=XH*AY(1,NN)
      BZ1=XKTZ1*AZ(1 MM)*DZ(N)
      AHZ=XH*AZ(1,MM)
      TOTCOEF=BX2+BY1+BZ1+AHY+AHZ
C     ENERGY FLOW DUE TO CONDUCTION
      CONDX=BX2*(2 MM,NN)
      CONDY=BY1*T(1 M NN)
      CONDZ=BZ1*T(1 MM N)
      TOTCOND=CONDX+CONDY+CONDZ
C     ENERGY FLOW DUE TO CONVECTION
      TOTCONV=(AHY+AHZ)*TA
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=RHO(1 MM,NN)*CP(1,MM NN)*
DV(1 MM NN)/DT
C     COMPUTE NEW NODE TEMPERATURE
      TMP=TOTCOND/COEFF+(1.0-TOTCOEF/COEFF)*
T(1,MM,NN)
      T(1),MM,NN)=TMP+(TOTCONV TOTHFG)/COEFF
      DELTA(1 MM NN)=T(1 MM NN)-T(1,MM,NN)
C     6  EXTERNAL NODE AT THE Y-Z INTERSECT
(LL,MM 1)
C     COMPUTE LATENT HEAT OF VAPORIZATION
      CALL XLHEAT(T(LL,MM,1)W(LL,MM 1),AW XL)
C     ENERGY FLOW DUE TO MOISTURE
VAPORIZATION
      HFGX(MM 1)=WLX(MM,1)*XL
      HFGY(LL,1)=WLY(LL,1)*XL
      TOTHFG=HFGX(MM,1)+HFGY(LL,1)
C     COMPUTE AVERAGE CONDUCTIVITY
      XKTX1=(XKT(1,MM 1)+XKT(LL,MM 1))/2.0
      XKTY1=(XKT(LL,M 1)+XKT(LL,MM 1))/2.0
      XKTZ2=(XKT(LL,MM,1)+XKT(LL,MM,2))/2.0
C     COMPUTE CONDUCTION & CONVECTION
COEFFICIENTS
      BX1=XKTX1*AX(MM,1)*DX(LL)
      AHX=XH*AX(MM,1)
      BY1=XKTY1*AY(LL,1)/DY(M)
      AHY=XH*AY(LL,1)
      BZ2=XKTZ2*AZ(LL,MM)*DZ(1)
      TOTCOEF=BX1+BY1+BZ2+AHX+AHY
C     ENERGY FLOW DUE TO CONDUCTION
      CONDX=BX1*T(1,MM,1)
      CONDY=BY1*T(LL,M 1)
      CONDZ=BZ2*T(LL,MM,2)
      TOTCOND=CONDX+CONDY+CONDZ
C     ENERGY FLOW DUE TO CONVECTION
      TOTCONV=(AHX+AHY)*TA
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=RHO(LL,MM 1)*CP(LL,MM 1)*
DV(LL,MM 1)/DT
C     COMPUTE NEW NODE TEMPERATURE
      TMP=TOTCOND/COEFF+(1.0-TOTCOEF/COEFF)*
T(LL,MM,1)
      T1(LL,MM,1)=TMP+(TOTCONV TOTHFG)/COEFF
      DELTA(LL,MM 1)=T1(LL,MM,1)-T(LL,MM,1)
C     7  EXTERNAL NODE AT THE Z-Y INTERSECT
(LL,1 NN)
C     COMPUTE LATENT HEAT OF VAPORIZATION
      CALL XLHEAT(T(LL,1,NN),W(LL 1 NN),AW XL)
C     ENERGY FLOW DUE TO MOISTURE
VAPORIZATION
      HFGX(1,NN)=WLX(1,NN)*XL
      HFGZ(LL 1)=WLZ(LL,1)*XL
      TOTHFG=HFGX(1 NN)+HFGZ(LL,1)
C     COMPUTE AVERAGE CONDUCTIVITY
      XKTX1=(XKT(L,1 NN)+XKT(LL 1,NN))/2.0
      XKTY2=(XKT(LL,1,NN)+XKT(LL,2,NN))/2.0
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     XKTZ1=(XKT(LL,1 N)+XKT(LL,1 NN))/2.0
C    COMPUTE CONDUCTION & CONVECTION
COEFFICIENTS
     BX1=XKTX1*AX(I,N%)/DX(L)
     AHX=XH*AX(I NN)
     BY2=XKTY2*AY(LL,NN)/DY(I)
     BZ1=XKZ1*%Z(LL,)/DZ(M)
     AHZ=%U*AZ(LL,1)
     TOTCOEF=BX1+BY2+BZ1+AHX+AHZ
C    ENERGY FLOW DUE TO CONDUCTION
     CONDX=BX1*T(L 1 NN)
     CONDY=BY2*T(LL,2,NN)
     CONDZ=-BZ1*T(LL,1 N)
     TOTCOND=CONDX+CONDY+CONDZ
C    ENERGY FLOW DUE TO CONVECTION
     TOTCONV=AHX-AHZ)*TA
C    COMPUTE TRANSIENT COEFFICIENT
     COEFF=-RHO(LL,1 NN)*CP(LL,1 NN)*
DV(LL,1 NN)/DT
C    COMPUTE NEW NODE TEMPERATURE
     TMP=TOTCOND/COEFF+(1 0-TOTCOEF/COEFF)*
T(LL,1,NN)
     T1(LL,1 NN)=TMP+(TOTCONV TOTHFG/COEFF
     DELTA(LL,1,NN)=T1(LL,1,NN)-T(LL,1 NN)
C    3--EXTERNAL CORNER OPPOSITE TO CENTER
(LL,MM,NN)
C    COMPUTE LATENT HEAT OF VAPORIZATION
     CALL
XLHEAT(T(LL,MM,NN),W(LL,MM,NN),AW,XL,)
C    ENERGY FLOW DUE TO MOISTURE
VAPORIZATION
     HFGX(MM,NN)=WLX(MM,NN)*XL
     HFGY(LL,NN)=WLY(LL,NN)*XL
     HFGZ(LL,MM)=WLZ(LL,MM)*XL
     TOTHFG=HFGX(MM,NN)+HFGY(LL,NN)+
HFGZ(LL,MM)
C    COMPUTE AVERAGE CONDUCTIVITY
     XKTX1=(XKT(LL MM NN)+XKT(LL MM,NN))/2 0
     XkTY1=(XKT(LL,M,NN)+XkT(LL,MM,NN))/2.0
     XKTZ1=(XKT(LL,MM,N)+XKT(LL,MM,NN))/2 0
C    COMPUTE CONDUCTION & CONVECTION
COEFFICIE NT*(
     BX1=XKTX1*AX(MM,NN)/DX(L)
     AHX=XH*AX(MM,NN)
     BY1=XkTY1*AY(LL,NN)/DY(M)
     AHY=XH*AY(LL,NN)
     BZ1=XKTZ1*AZ(I LMM)/DZ(N)
     AHZ=XH*AZ(LL,MM)
     TOTCOEF=BX1+BY1+BZ1+AHX+AHY+AHZ
C    ENERGY FLOW DUE TO CONDUCTION
     CONDX=BX1*T(L 1 MM,NN)+BX1*T(I LMM NN)
     CONDY=-BY1*T(LL,M,NN)
     CONDZ=-BZ1*T(LL,MM,N)
     TOTCOND=CONDX+CONDY+CONDZ
C    ENERGY FLOW DUE TO CONVECTION
     TOTCONV=-AHX+AHY+AHZ)*TA
C    COMPUTE TRANSIENT COEFFICIENT
     COEFF=-RHO(LMM,NN)*CP(LMM,NN)*
DV(I MM,NN)/DT
C    COMPUTE NEW NODE TEMPERATURE
     TMP=TOTCOND/COEFF+(1 0-TOTCOEF/COEFF)*
T(LMM,NN)
     T1(LMM,NN)=TMP+(TOTCONV TOTHFG/COEFF
     DELTA(LMM,NN)=T1(LMM,NN)-T(LMM,NN)
     DO I=2,L
C    2--EXTERNAL EDGE (CONVECTION)
(LMM,NN)
C    COMPUTE LATENT HEAT OF VAPORIZATION
     CALL XLHEAT(T(LMM,NN),W(LMM,NN),AW,XL)
C    ENERGY FLOW DUE TO MOISTURE
VAPORIZATION
     HFGY(I NN)=WLY(I NN)*XL
     HFGZ(LMM)=WLZ(LMM)*XL
     TOTHFG=HFGY(I NN)+HFGZ(I MM)
C    COMPUTE AVERAGE CONDUCTIVITY
     XkTX1=(XKT(I LMM,NN)+XkT(LMM,NN))/2 0
     XkTX2=(XkT(I MM,NN)+Xk.T(I+1 MM,NN))/2.0
     XKTY1=(XKT(I M,NN)+XkT(I MM 1))/2 0
     XKTY2=(XKT(I M 1)+XkT(I MM 1))/2 0
     XKTZ1=(XKT(I MM,N)+XkT(I MM NN))/2 0
     XKTZ2=(XkT(I MM,1)+XkT(I MM,2))/2.0
C    COMPUTE CONDUCTION & CONVECTION
COEFFICIENTS
     BX1=XkTX1*AX(MM,NN)/DX(I+1)
     BX2=XKTX2*AX(MM,NN)/DX(I)
     BY1=XkTY1*AY(LNN)/DY(M)
     AHY=XH*AY(I,NN)
     BZ1=XkTZ1*AZ(I,MM)/DZ(N)
     AHZ=XH*AZ(I,MM)
     TOTCOEF=BX1+BX2+BY1+BZ1+AHY+AHZ
C    ENERGY FLOW DUE TO CONDUCTION
     CONDX=BX1*T(I+1 MM,NN)+BX2*T(I+1,MM NN)
     CONDY=BY1*T(I M,NN)
     CONDZ=BZ1*T(I,MM,N)
     TOTCOND=CONDX+CONDY+CONDZ
C    ENERGY FLOW DUE TO CONVECTION
     TOTCONV=-AHY+AHZ)*TA
C    COMPUTE TRANSIENT COEFFICIENT
     COEFF=-RHO(LMM,NN)*CP(LMM,NN)*
DV(I MM,NN)/DT
C    COMPUTE NEW NODE TEMPERATURE
     TMP=TOTCOND/COEFF+(1 0-TOTCOEF/COEFF)*
T(LMM,NN)
     T1(LMM,NN)=TMP+(TOTCONV TOTHFG/COEFF
     DELTA(LMM,NN)=T1(I MM NN)-T(I MM NN)
   END DO          ! *** end of I do loop ***
   DO I=2,L
C    3--EDGE OF SYMMETRY & CONVECTION
(LMM 1)
C    COMPUTE LATENT HEAT OF VAPORIZATION
     CALL XLHEAT(T(LMM 1),W(LMM,1),AW,XL)
C    ENERGY FLOW DUE TO MOISTURE
VAPORIZATION
     HFGY(I 1)=WLY(I 1)*XL
     TOTHFG=HFGY(I 1)
C    COMPUTE AVERAGE CONDUCTIVITY
     XKTX1=(XkT(I LMM 1)+XkT(I MM 1))/2.0
     XKTX2=(XkT(I,MM,1)+XkT(I+1 MM,1))/2.0
     XkTY1=(XKT(I M 1)+XkT(I MM 1))/2 0
     XKTZ2=(XkT(I MM,1)+XkT(I,MM,2))/2.0
C    COMPUTE CONDUCTION & CONVECTION
COEFFICIENTS
     BX1=XKTX1*AX(MM )/DX(I 1)
     BX2=XKTX2*AX(MM )/DX(I)
     BY1=XkTY1*AY(I )/DY(M)
     AHY=XH*AY(I 1)
     BZ2=XKTZ2*AZ(LMM)/DZ(1)
     TOTCOEF=BX1+BX2+BY1+BZ2+AHY
C    ENERGY FLOW DUE TO CONDUCTION
     CONDX=BX1*T(I 1,MM,1)+BX2*T(I+1,MM 1)
     CONDY=-BY1*T(I M,1)
     CONDZ=-BZ2*T(LMM,2)
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      TOTCOND=CONDX+CONDY+CONDZ
C     ENERGY FLOW DUE TO CONVECTION
      TOTCONV= AHY*TA
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF= RHO(LMM,1)*CP(LMM,1)*DV(LMM,1)/DT
C     COMPUTE NEW NODE TEMPERATURE
      TMP=TOTCOND/COEFF+(1.0-TOTCOEF/COEFF)*
T(LMM,1)
      T1(LMM,1)=TMP+(TOTCONV-TOTHFG)/COEFF
      DELTA(LMM,1)=T1(LMM,1)-T(LMM,1)
      END DO          ! *** end of I do loop ***
      DO J=2,L
C     4-- EDGE OF SYMMETRY & CONVECTION
(I,1,N)
C     COMPUTE LATENT HEAT OF VAPORIZATION
      CALL XLHEAT(T(I,1,N),W(I,1,N),AW,XL)
C     ENERGY FLOW DUE TO MOISTURE
VAPORIZATION
      HFGZ(I,1)=WLZ(I,1)*XL
      TOTHFG=HFGZ(1)
C     COMPUTE AVERAGE CONDUCTIVITY
      XKTX1=(XKT(I-1,1,N)+XKT(I,1,N))/2.0
      XKTX2=(XKT(I,1,N)+XKT(I+1,1,N))/2.0
      XKTY2=(XKT(I,1,N)+XKT(I,2,N))/2.0
      XKTZ1=(XKT(I,1,N)+XKT(I,1,N))/2.0
C     COMPUTE CONDUCTION & CONVECTION
COEFFICIENTS
      BX1=XKTX1*AX(I,1,N)/DX(I-1)
      BX2=XKTX2*AX(I,1,N)/DX(I)
      BY2=XKTY2*AY(I,1,N)/DY(1)
      BZ1=XKTZ1*AZ(I,1)/DZ(N)
      AHZ=XH*AZ(I,1)
      TOTCOEF=BX1+BX2+BY2+BZ1+AHZ
C     ENERGY FLOW DUE TO CONDUCTION
      CONDX=BX1*T(I-1,1,N)+BX2*T(I+1,1,N)
      CONDY=BY2*T(I,2,N)
      CONDZ=BZ1*T(I,1,N)
      TOTCOND=CONDX+CONDY+CONDZ
C     ENERGY FLOW DUE TO CONVECTION
      TOTCONV=AHZ*TA
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=RHO(I,1,N)*CP(I,1,N)*DV(I,1,N)/DT
C     COMPUTE NEW NODE TEMPERATURE
      TMP=TOTCOND/COEFF+(1.0-TOTCOEF/COEFF)*
T(I,1,N)
      T1(I,1,N)=TMP+(TOTCONV-TOTHFG)/COEFF
      DELTA(I,1,N)=T1(I,1,N)-T(I,1,N)
      END DO          ! *** end of I do loop ***
      DO J=2,M
C     6-- EXTERNAL EDGE (CONVECTION)-- (1,L,J,N)
C     COMPUTE LATENT HEAT OF VAPORIZATION
      CALL XLHEAT(T(1,L,J,N),W(1,L,J,N),AW,XL)
C     ENERGY FLOW DUE TO MOISTURE
VAPORIZATION
      HFGX(1,N)=WLX(1,N)*XL
      HFGZ(1,L,J)=WLZ(1,L,J)*XL
      TOTHFG=HFDX(1,N)+HFGZ(1,L,J)
C     COMPUTE AVERAGE CONDUCTIVITY
      XKTX1=(XKT(1,J,N)+XKT(1,L,J,N))/2.0
      XKTY1=(XKT(1,L,J,N)+XKT(1,L,J,N))/2.0
      XKTY2=(XKT(1,L,J,N)+XKT(1,L+1,J,N))/2.0
      XKTZ1=(XKT(1,L,J,N)+XKT(1,L,J,N))/2.0
C     COMPUTE CONDUCTION & CONVECTION
COEFFICIENTS
      BX1=XKTX1*AX(1,N)/DX(1)
      AHX=XH*AX(1,N)
      BY1=XKTY1*AY(1,L,N)/DY(J-1)
      BY2=XKTY2*AY(1,L,N)/DY(J)
      BZ1=XKTZ1*AZ(1,L,J)/DZ(N)
      AHZ=XH*AZ(1,L,J)
      TOTCOEF=BX1+BY1+BY2+BZ1+AHX+AHZ
C     ENERGY FLOW DUE TO CONDUCTION
      CONDX=BX1*T(2,L,J,N)
      CONDY=BY1*T(1,L-1,J,N)+BY2*T(1,L+1,J,N)
      CONDZ=BZ1*T(1,L,J,N)
      TOTCOND=CONDX+CONDY+CONDZ
C     ENERGY FLOW DUE TO CONVECTION
      TOTCONV=AHZ*TA
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=RHO(1,J,N)*CP(1,J,N)*DV(1,J,N)/DT
C     COMPUTE NEW NODE TEMPERATURE
      TMP=TOTCOND/COEFF+(1.0-TOTCOEF/COEFF)*
T(1,J,N)
      T1(1,J,N)=TMP+(TOTCONV-TOTHFD)/COEFF
      DELTA(1,J,N)=T1(1,J,N)-T(1,J,N)
      END DO          ! *** end of I do loop ***
      DO I=2,M
C     8--EDGE OF SYMMETRY & CONVECTION
(I,L,J,1)
C     COMPUTE LATENT HEAT OF VAPORIZATION
      CALL XLHEAT(T(I,L,J,1),W(I,L,J,1),AW,XL)
C     ENERGY FLOW DUE TO MOISTURE
VAPORIZATION
      HFGZ(I,J)=WLZ(I,J)*XL
      TOTHFG=HFGZ(I,J)
C     COMPUTE AVERAGE CONDUCTIVITY
      XKTX2=(XKT(I,L,J,N)+XKT(2,L,J,N))/2.0
      XKTY1=(XKT(I,L-1,J,N)+XKT(I,L,J,N))/2.0
      XKTY2=(XKT(I,L,J,N)+XKT(I,L+1,J,N))/2.0
      XKTZ1=(XKT(I,L,J,N)+XKT(I,L,J,N))/2.0
C     COMPUTE CONDUCTION & CONVECTION
COEFFICIENTS
      BX2=XKTX2*AX(I,N)/DX(1)
      BY1=XKTY1*AY(I,N)/DY(L-1)
      BY2=XKTY2*AY(I,N)/DY(L)
      BZ1=XKTZ1*AZ(I,J)/DZ(N)
      AHZ=XH*AZ(I,J)
      TOTCOEF=BX2+BY1+BY2+BZ1+AHZ
C     ENERGY FLOW DUE TO CONDUCTION
      CONDX=BX2*T(2,J,N)
      CONDY=BY1*T(I,L-1,N)+BY2*T(I,L+1,N)
      CONDZ=BZ1*T(I,L,J,N)
      TOTCOND=CONDX+CONDY+CONDZ
C     ENERGY FLOW DUE TO CONVECTION
      TOTCONV=AHZ*TA
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=RHO(I,J,N)*CP(I,J,N)*DV(I,J,N)/DT
C     COMPUTE NEW NODE TEMPERATURE
      TMP=TOTCOND/COEFF+(1.0-TOTCOEF/COEFF)*
T(I,J,N)
      T1(I,J,N)=TMP+(TOTCONV-TOTHFD)/COEFF
      DELTA(I,J,N)=T1(I,J,N)-T(I,J,N)
      END DO          ! *** end of I do loop ***
      DO I=2,M
C     8--EDGE OF SYMMETRY & CONVECTION
(I,L,J,1)
C     COMPUTE LATENT HEAT OF VAPORIZATION
      CALL XLHEAT(T(I,L,J,1),W(I,L,J,1),AW,XL)
C     ENERGY FLOW DUE TO MOISTURE
VAPORIZATION
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      HFGX(I,J)=WLX(I,J)*XL
      TOTHFG=HFGX(I,J)
C     COMPUTE AVERAGE CONDUCTIVITY
      XKTX1=(XKT(I,J-1)+XKT(I,L,J-1))/2.0
      XKTY1=(XKT(I,L,J-1)+XKT(I,L,J))/2.0
      XKTY2=(XKT(I,L,J)+XKT(I,L,J+1))/2.0
      XKTZ2=(XKT(I,L,J)+XKT(I,L,J))/2.0
C     COMPUTE CONDUCTION & CONVECTION
COEFFICIENTS
      BX1=XKTX1*AX(I,J)/DX(L)
      AHX=XH*AX(I,J)
      BY1=XKTY1*AY(I,L,J)/DY(J-1)
      BY2=XKTY2*AY(I,L,J)/DY(J)
      BZ2=XKTZ2*AZ(I,L,J)/DZ(L)
      TOTCOLF=BX1+BY1+BY2+BZ2+AHX
C     ENERGY FLOW DUE TO CONDUCTION
      CONDX=BX1*T(L,J-1)
      CONDY=BY1*T(I,L,J-1)+BY2*T(I,L,J+1)
      CONDZ=BZ2*T(I,L,J2)
      TOTCOND=CONDX+CONDY+CONDZ
C     ENERGY FLOW DUE TO CONVECTION
      TOTCONV=AHX*TA
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=RHO(I,J,L)*CP(I,L,J)*DV(I,L,J)/DT
C     COMPUTE NEW NODE TEMPERATURE
      TMP=TOTCOND/COEFF+(1.0-TOTCOEF/COEFF)*
T(I,L,J)
      T(I,L,J)=TMP+(TOTCONV-TOTHFG)/COEFF
      DELTA(I,L,J)=T(I,L,J)-T(I,L,J)
    END DO          ! *** end of J do loop ***
    DO K=2,N
C   II   EXTERNAL EDGE (CONVECTION)
(I,L,MM,K)
C     COMPUTE LATENT HEAT OF VAPORIZATION
      CALL XLHEAT(T(I,L,MM,K),WI(I,L,MM,K),AW,XL)
C     ENERGY FLOW DUE TO MOISTURE
VAPORIZATION
      HFGX(MM,K)=WLX(MM,K)*XL
      HFGY(I,L,K)=WLY(I,L,K)*XL
      TOTHFG=HFGX(MM,K)+HFGY(I,L,K)
C     COMPUTE AVERAGE CONDUCTIVITY
      XKTX1=(XKT(I-MM,K)+XKT(I,MM,K))/2.0
      XKTY1=(XKT(I,L,M,K)+XKT(I,L,MM,K))/2.0
      XKTZ1=(XKT(I,L,MM,K-1)+XKT(I,L,MM,K))/2.0
      Xk.TZ=(Xk.K(I,L,MM,).+Xk.T(I,L,MM,K-1))/2.0
C     COMPUTE CONDUCTION & CONVECTION
COEFFICIENTS
      BX1=XKTX1*AX(MM,K)/DX(L)
      AHX=XH*AX(MM,K)
      BY1=XKTY1*AY(I,L,K)/DY(M)
      AHY=XH*AY(I,L,K)
      BZ1=XkTZ1*AZ(I,L,MM)/DZ(K-1)
      BZ2=XKTZ..*AZ(I,L,MM)/DZ(K)
      TOTCOEF=BX1+BY1+BZ1+BZ2+AHX+AHY
C     ENERGY FLOW DUE TO CONDUCTION
      CONDX=BX1*T(L,MM,K)
      CONDY=BY1*T(LL,M,K)
      CONDZ=BZ1*T(LL,MM K 1)+BZ2*T(LL,MM,K+1)
      TOTCOND=CONDX+CONDY+CONDZ
C     ENERGY FLOW DUE TO CONVECTION
      TOTCONV=AHX+AHY*TA
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=RHO(LL,MM K)*CP(LL,MM,K)*
DV(LL,MM K)/DT
C     COMPUTE NEW NODE TEMPERATURE
      TMP=TOTCOND/COEFF+(1.0-TOTCOEF/COEFF)*
T(LL,MM K)
      T(LL,MM,K)=TMP+(TOTCONV-TOTHFG)/COEFF
      DELTA(LL,MM,K)=T(LL,MM,K)-T(LL,MM,K)
    END DO          ! *** end of K do loop ***
    DO K=2,N
C   II   EDGE OF SYMMETRY & CONVECTION
(I,MM,K)
C     COMPUTE LATENT HEAT OF VAPORIZATION
      CALL XLHEAT(T(I,MM K) WI(I MM,K),AW XL)
C     ENERGY FLOW DUE TO MOISTURE
VAPORIZATION
      HFGY(I,K)=WLY(I K)*XL
      TOTHFG=HFGY(I,K)
C     COMPUTI. AVERAGE CONDUCTIVITY
      XkTX2=(Xk.T(I MM,K)+XkT(2,MM,K))/2.0
      XKTY1=(XKT(I M K)+XKT(I MM K))/2.0
      XKTZ1=(XKTI I MM K.1)+XKT(I MM,K))/2.0
      XKTY2=(XKT(I,MM,K)+XKT(I,MM K+1))/2.0
C     COMPUTE CONDUCTION & CONVECTION
COEFFICIINTS
      BX2=XKTX2*AX(MM,K)/DX(1)
      BY1=XKTY1*AY(I K)DY(M)
      AHY=XH*AY(I K)
      BZ1=XKTZ1*AZ(I MM)/DZ(K 1)
      BZ2=XKTZ2*AZ(I MM)/DZ(K)
      TOTCOEF=BX2+BY1+BZ1+BZ2+AHY
C     ENLBGY FLOW DUL TO CONDUCTION
      CONDX=BX2*T(2 MM,K)
      CONDY=BY1*T(I M,K)
      CONDZ=BZ1*T(LL,MM,K-1)+BZ2*T(I,MM,K+1)
      TOTCOND=CONDX+CONDY+CONDZ
C     ENPRGY FLOW DUE TO CONVECTION
      TOTCONV=AHY*TA
C     COMPUTI TRANSIENT COEFFICIENT
      COEFF=RHO(I MM K)*CP(I MM,K)*
DV(I,MM K)/DT
C     COMPLTE NEW NODE TEMPERATURE
      TMP=TOTCOND/COEFF+(1.0-TOTCOEF/COEFF)*
T(LL,MM K)
      T(LL MM,K)=TMP+(TOTCONV-TOTHFG)/COEFF
      DELTA(LL,MM,K)=T(LL,MM,K)-T(LL,MM,K)
    END DO          ! *** end of K do loop ***
    DO K=2,N
C   II   EDGE OF SYMMETRY & CONVECTION
(LL,.) K)
C     COMPUTL LATENT HEAT OF VAPORIZATION
      CALL XLHEAT(T(LL.I,K) WI(L.I K),AW XL)
C     ENERGY FLOW DUE TO MOISTURE
VAPORIZATION
      HFGX(1 K)=WLX(1 K)*XL
      TOTHFG=HFGX(1,K)
C     COMPUTI AVTRAGE CONDUCTIVITY
      XkTX1=(XKT(LL.I,K)+XKT(LL.I K))/2.0
      XKTY2=(XKT(LL.I.K)+XkTI L.2 K))/2.0
      XKTZ1=(XKT(LL.I.K-1)+XKT(LL.I K))/2.0
      XKTZ2=(XKT(LL.I.K)+XKT(LL.I,K+1))/2.0
C     COMPUTE CONDUCTION & CONVECTION
COEFFICIINTS
      BX1=XkTX1*AX(1,K)/BX(L)
      AHX=XH*AX(I,K)
      BY2=XKTY2*AY(LL,K)/DY(I)
      BZ1=XKTZ1*AZLL I)/DZ(K 1)
      BZ2=XkTZ2*AZ(LL I)/DZ(K)
      TOTCOEF=BX1+BY2+BZ1+BZ2+AHX
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C     ENERGY FLOW DUE TO CONDUCTION
      CONDX=BX1*T(L,I,K)
      CONDY=BY2*T(L,I-2,K)
      CONDZ=BZ1*T(L,I,K-1)+BZ2*T(L,I,K+1)
      TOTCOND=CONDX+CONDY+CONDZ
C     ENERGY FLOW DUE TO CONVECTION
      TOTCONV=AHX*TA
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=RHO(L,I,K)*CP(L,I,K)*DV(I,L,K)/DT
C     COMPUTE NEW NODE TEMPERATURE
      TMP=TOTCOND/COEFF+(1.0-TOTCOEF/COEFF)*
T(L,I,K)
      T(L,I,I,K)=TMP+(TOTCONV TOTHFG)/COEFF
      DELTA(L,I,K)=T(L,I,K)-T(L,I,K)
      END DO          ! *** end of K do loop ***
      DO I=2,I,
      DO J=2,M
C     2-EXTERNAL SURFACE XY-(I,J,NN)
C     COMPUTE LATENT HEAT OF VAPORIZATION
      CALL XLHEAT(T(I,J,NN) WH,J,NN),AW XL)
C     ENERGY FLOW DUE TO MOISTURE
VAPORIZATION
      HFGF(I,J)=WL2(I,J)*XL
      TOTHFG=HFGZ(I,J)
C     COMPUTE AVERAGE CONDUCTIVITY
      XKTX1=(XKT(I-1,J,NN)+XKT(I,J,NN))/2.0
      XKTX2=(XKT(I,J,NN)+XKT(I+1,J,NN))/2.0
      XKTY1=(XKT(I,J-1,NN)+XKT(I,J,NN))/2.0
      XKTY2=(XKT(I,J,NN)+XKT(I,J+1,NN))/2.0
      XKTZ1=(XKT(I,J,NN)+XKT(I,J,K-1))/2.0
      XKTZ2=(XKT(I,J,NN)+XKT(I,J,K+1))/2.0
C     COMPUTE CONDUCTION & CONVECTION
COEFFICIENTS
      BX1=XKTX1*AX(J,NN)/DX(I-1)
      BX2=XKTX2*AX(J,NN)/DX(I)
      BY  =XKTY1*AY(I,NN)DY(J-1)
      BY2=XKTY2*AY(I,NN)/DY(J)
      BZ1=XKTZ1*AZ(I,J)DZ(N)
      AHZ=XI)*AZ(I,J)
      TOTCOEF=BX1+BX2+BY1+BY2+BZ1+AHZ
C     ENERGY FLOW DUE TO CONDUCTION
      CONDX=BX1*T(L,I,NN)+BX2*T(I+1,NN)
      CONDY=BY1*T(L,I,NN)+BY2*T(J+1,NN)
      CONDZ=BZ1*T(L,I,NN)
      TOTCOND=CONDX+CONDY+CONDZ
C     ENERGY FLOW DUE TO CONVECTION
      TOTCONV=AHZ*TA
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=RHO(L,I,NN)*CP(L,I,NN)*DV(L,NN)/DT
C     COMPUTE NEW NODE TEMPERATURE
      TMP=TOTCOND/COEFF+(1.0-TOTCOEF/COEFF)*
T(I,J,NN)
      T(I,J,I,NN)=TMP+(TOTCONV TOTHFG)/COEFF
      DELTA(I,J,NN)=T(I,J,NN)-T(I,J,NN)
      END DO          ! *** end of I-J do loops ***
      DO I=2,M
      DO K=2,N
C     4-EXTERNAL SURFACE YZ-(L,I,J,K)
C     COMPUTE LATENT HEAT OF VAPORIZATION
      CALL XLHEAT(T(L,I,K) W(L,I,K),AW XL)
C     ENERGY FLOW DUE TO MOISTURE
VAPORIZATION
      HFGK(I,K)=WL3(I,K)*XL
      TOTHFG=HFGX(I,K)
C     COMPUTE AVERAGE CONDUCTIVITY
      XKTX1=(XKT(I-1,K)+XKT(I,I,K))/2.0
      XKTY1=(XKT(I,I-1,K)+XKT(I,I,K))/2.0
      XKTY2=(XKT(I,I,K)+XKT(I,I+1,K))/2.0
      XKTZ1=(XKT(I,I,K-1)+XKT(I,I,K))/2.0
      XKTZ2=(XKT(I,I,K)+XKT(I,I,K+1))/2.0
C     COMPUTE CONDUCTION & CONVECTION
COEFFICIENTS
      BX1=XKTX1*AX(MM,K)/DX(I-1)
      BX2=XKTX2*AX(MM,K)/DX(I)
      BY1=XKTY1*AY(I,K)/DY(M)
      AHY=XI*AY(I,K)
      BZ1=XKTZ1*AZ(MM)DZ(K-1)
      BZ2=XKTZ2*AZ(LMM)DZ(K)
      TOTCOEF=BX1+BX2+BY1+BZ1+BZ2+AHY
C     ENERGY FLOW DUE TO CONDUCTION
      CONDX=BX1*T(I-1,MM,K)+BX2*T(I+1,MM,K)
      CONDY=BY1*T(LMM,K)
      CONDZ=BZ1*T(LMM,K-1)+BZ2*T(LMM,K+1)
      TOTCOND=CONDX+CONDY+CONDZ
C     ENERGY FLOW DUE TO CONVECTION
      TOTCONV=AHY*TA
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=RHO(L,I,K)*CP(L,I,K)*DV(L,I,K)/DT
C     COMPUTE NEW NODE TEMPERATURE
      TMP=TOTCOND/COEFF+(1.0-TOTCOEF/COEFF)*
T(L,I,K)
      T(L,I,I,K)=TMP+(TOTCONV TOTHFG)/COEFF
      DELTA(L,I,K)=T(L,I,K)-T(L,I,K)
      END DO          ! *** end of I-K do loops ***
CCCCC
      DO I=2,I,
      DO K=2,N
C     6-EXTERNAL SURFACE XZ-(I MM,K)
C     COMPUTE AVERAGE CONDUCTIVITY
      CALL XLHEAT(TI,MM,K),W(I,MM,L),AW XL)
C     ENERGY FLOW DUE TO MOISTURE
VAPORIZATION
      HFGY(I,K)=WLY(I,K)*XL
      TOTHI G=HFGY(I,K)
C     COMPUTE AVERAGE CONDUCTIVITY
      XkTX1=(XkT(I-1 MM,k)+XkT(I,MM K))/2.0
      XKTX2=(XKT(I-MM k)+XKT(I+1 MM,K))/2.0
      XKTY1=(XkT(I MM,k)+XkT(I,MM,K))/2.0
      XKTZ1=(XkT(I,MM,k-1)+XkT(I MM,K))/2.0
      XkTZ2=(XKT(I MM,k)+XkT(I MM,k-1))/2.0
C     COMPUTE CONDUCTION & CONVECTION
COEFFICIENTS
      BX1=XkTX1*AX(MM,K)/DX(I-1)
      BX2=XKTX2*AX(MM,K)/DX(I)
      BY1=XkTY1*AY(I K)/DY(M)
      AHY=XI*AY(I,K)
      BZ1=XkTZ1*AZ(LMM)DZ(K-1)
      BZ2=XKTZ2*AZ(LMM)DZ(k)
      TOTCOEF=BX1+BX2+BY1+BZ1+BZ2+AHY
C     ENERGY FLOW DUL TO CONDUCTION
      CONDX=BX1*T(I-1 MM,k)+BX2*T(I+1 MM,K)
      CONDY=BY1*T(LMM,K)
      CONDZ=BZ1*T(LMM,K-1)+BZ2*T(LMM,K+1)
      TOTCOND=CONDX+CONDY+CONDZ
C     ENERGY FLOW DUE TO CONVECTION
      TOTCONV=AHY*TA
C     COMPUTE TRANSIENT COEFFICIENT
COEFF=HHO(LMM K)*CP0 MM k)*DV(LMM,K)/DT
C     COMPUTE NEW NODE TEMPERATURE
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      TMP=TOTCOND/COEFF+(1.0-TOTCOEF/COEFF)*
T(I,MM,K)
      T(I,MM,K)=TMP+(TOTCONV-TOTHFG)/COEFF
      DELTA(I,MM,K)=T(I,MM,K)-T(I,MM,K)
      END DO
    END DO          ! *** end of I-K do loops ***
    RETURN
    END
C*****************************************************
    SUBROUTINE ACID3(NAC_BC,TIME,DT,L,M,N)
C*****************************************************
C   SUBROUTINE TO CALCULATE ACETIC ACID C
C   CONCENTRATION DISTRIBUTION
C   IN TIME AND SPACE DURING CACA DRYING
C  KQ NOMENCLATURE OF VARIABLES
C I  AC_BC    ACETIC ACID CONCENTRATION AT C
C   THE BOUNDARY NODES (DECIMAL, DRY BASIS)
C I  TIME     ELAPSED TIME (S)
C I  DT       TIME INCREMENT (S)
C I  I        INDEX FOR SPACE IN THE X DIRECTION
C I  J        INDEX FOR SPACE IN THE Y DIRECTION
C I  K,       INDEX FOR SPACE IN THE Z DIRECTION
C I  L        NO OF SUBINTERVALS -X DIRECTION
C I  M,       NO OF SUBINTERVALS -Y DIRECTION
C I  N        NO OF SUBINTERVALS -Z DIRECTION
C  O C_       ACETIC ACID CONC (DEC_DB)
C  W_         MOISTURE CONTENT (DECIMAL, D B )
C  T          NODE TEMPERATURE (C)
C  DIFF       ACID ACETIC DIFFUSIVITY (M2/S)
C  RHOD       DENSITY OF DRY BONE MATERIAL
(KG/M3)
C***************************************************
    DIMENSION DIFF(15,15,15)
    COMMON /TEMP/  T(15,15,15),T1(15,15,15)
    COMMON /MOIST/  W(15,15,15),W1(15,15,15)
    COMMON /ACID/  C(15,15,15),C1(15,15,15)
    COMMON  SPGRID/ X(15),Y(15),Z(15),DX(15),
DY(15),DZ(15),AX(15,15),AY(15,15),AZ(15,15),
DV(15,15,15)
C***************************************************
C   COMPUTE NUMBER OF NODES
      LL=L+1
      MM=M+1
      NN=N+1
C   COMPUTE DENSITY OF DRY BONE MATERIAL
      IF(TIME.EQ.0.0) THEN
        WW=0.0
        CALL
SIZE(WW,IUN,IRY,IRZ,A,VOL,XMASS,RHOD)
      ELSE
      ENDIF
C   COMPUTE MOISTURE DIFF. DIFF(I,J,K)
    DO I=1,LL
      DO J=1,MM
        DO K=1,NN
          CALL DIFFAC(T(I,J,K),W(I,J,K),DIFF(I,J,K))
        END DO
      END DO
    END DO
CCCCC
C   CORNER ELEMENT VOLUMES (8)
C   1  CENTER NODE. ORIGIN OF COORD. SYSTEM
(I,J,1)
C COMPUTE AVERAGE DIFFUSIVITY  NODES I & I+1
      DIFFAX2=(DIFF(I,J,1)+DIFF(2,J,1))/2.0
C   COMPUTE AV. DIFFUSIVITY  NODES J & J+1
      DIFFAY2=(DIFF(I,J,1)+DIFF(I,2,1))/2.0
C   COMPUTE AV. DIFFUSIVITY  NODES K & K+1
      DIFFAZ=-(DIFF(I,J,1)+DIFF(I,J,2))/2.0
C   COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX2=DIFFAX2*AX(I,1)/DX(1)
      BY2=DIFFAY2*AY(I,1)/DY(1)
      BZ2=DIFFAZ2*AZ(I,1)/DZ(1)
      DIFFCOEF=BX2+BY2+BZ2
C   COMPUTE ACETIC ACID FLOW DUE TO
DIFFUSION
      ADIFFX=BX2*C(2,I,1)
      ADIFFY=BY2*C(I,2,1)
      ADIFFZ=BZ2*C(I,I,2)
      TOTDIFF=ADIFFX+ADIFFY+ADIFFZ
C   COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(I,I,1)/DT
C   COMPUTE NEW ACETIC ACID
CONCENTRATION
      AMP=TOTDIFF/COEFF+() 0-DIFFCOEF/COEFF)*
C(I,I,1)
      C1(I,I,1)=AMP
C   SURFACE NODES - IMPOSED BOUNDARY
CONDITION
C   2  EXTERNAL NODE AT THE END OF X EDGE
(LL,I,1)
      C1(LL,I,1)=AC_BC
C   3--EXTERNAL NODE AT THE END OF Y EDGE
(I,MM,1)
      C1(I,MM,1)=AC_BC
C   4--EXTERNAL NODE AT THE END OF Z EDGE
(I,I,NN)
      C1(I,I,NN)=AC_BC
C   5--EXTERNAL NODE AT THE Y-Z INTERSECT
(LL,MM,NN)
      C1(LL,MM,NN)=AC_BC
C   6  EXTERNAL NODE AT THE Y-Z INTERSECT
(LL,MM,1)
      C1(LL,MM,1)=AC_BC
C   7  EXTERNAL NODE AT THE Z-Y INTERSECT
(LL,I,NN)
      C1(LL,I,NN)=AC_BC
C   8--EXTERNAL CORNER OPPOSITE TO CENTER
(LL,MM,NN)
      C1(LL,MM,NN)=AC_BC
C   NODES ALONG THE SLAB EDGES (12)
C   EDGES OF SYMMETRY (INSULATION)
C   1--EDGE(1,1,1)
    DO I=2,L
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFAX1=(DIFF(I-1,1,1)+DIFF(I,1,1))/2.0
      DIFFAX2=(DIFF(I,1,1)+DIFF(I+1,1,1))/2.0
      DIFFAY2=(DIFF(I,1,1)+DIFF(I,2,1))/2.0
      DIFFAZ2=(DIFF(I,1,1)+DIFF(I,1,2))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      BX1=DIFFAX1*AX(I,1)/DX(I,1)
      BX2=DIFFAX2*AX(I,1)/DX(I)
      BY2=DIFFAY2*AY(I,1)/DY(1)
      BZ2=DIFFAZ2*AZ(I,1)/DZ(1)
      DIFFCOEF=BX1+BX2+BY2+BZ2
C     COMPUTE ACETIC ACID FLOW DUE TO
DIFFUSION
```

```
      ADIFFX=0X1*C(0,1,1)+0X2*C(0+1,1,1)
      ADIFFY=0Y2*C(0,2,1)
      ADIFFZ=0Z2*C(0,1,2)
      TOTDIFF=ADIFFX+ADIFFY+ADIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(I,J,1)/DT
C     COMPUTE NEW ACETIC ACID
CONCENTRATION
      AMP=TOTDIFF/COEFF+(1.0-DIFFCOEF/COEFF)*
C(I,J,1)
      C1(I,J,1)=AMP
C     SURFACE NODES  IMPOSED BOUNDARY
CONDITION
C     EXTERNAL EDGES (CONVECTION)
C     EDGES WITH INSULATION & CONVECTION
C     2  EDGE(I,1,MM,NN)
C     3  EDGE(I,MM,1)
C     4  EDGE(I,1,NN)
      C1(I,MM,NN)=AC_BC
      C1(I,MM,1)=AC_BC
      C1(I,1,NN)=AC_BC
      END DO
C     5  EDGE(I,J,1)
      DO J=2,N1
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFAX2=(DIFF(I,J,1)+DIFF(2,J,1))/2.0
      DIFFAY1=(DIFF(I,J,1)+DIFF(I,J,1))/2.0
      DIFFAY2=(DIFF(I,J,1)+DIFF(I,J+1,1))/2.0
      DIFFAZ2=(DIFF(I,J,1)+DIFF(I,J,2))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      0X2=DIFFAX2*AX(I,J)*DX(1)
      0Y1=DIFFAY1*AY(I,J)*DY(I)
      0Y2=DIFFAY2*AY(I,J)*DY(J)
      0Z2=DIFFAZ2*AZ(I,J)*DZ(1)
      DIFFCOEF=0X2+0Y1+0Y2+0Z2
C     COMPUTE ACETIC ACID FLOW DUE TO
DIFFUSION
      ADIFFX=0X2*C(2,1,1)
      ADIFFY=0Y2*C(I,2,1)
      ADIFFZ=0Z2*C(I,1,2)
      TOTDIFF=ADIFFX+ADIFFY+ADIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(I,J,1)/DT
C     COMPUTE NEW ACETIC ACID
CONCENTRATION
      AMP=TOTDIFF/COEFF+(1.0-DIFFCOEF/COEFF)*
C(I,J,1)
      C1(I,J,1)=AMP
C     SURFACE NODES  IMPOSED BOUNDARY
CONDITION
C     EXTERNAL EDGES (CONVECTION)
C     EDGES WITH INSULATION & CONVECTION
C     6  EDGE(I,1,NN)
C     7  EDGE(I,MM,NN)
C     8  EDGE(I,1,1)
      C1(I,1,NN)=AC_BC
      C1(I,MM,NN)=AC_BC
      C1(I,1,1)=AC_BC
      END DO
C     9  EDGE(1,I,K)
      DO K=2,N
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFAX2=(DIFF(1,I,K)+DIFF(2,I,K))/2.0
      DIFFAY2=(DIFF(1,I,K)+DIFF(1,2,K))/2.0
      DIFFAZ1=(DIFF(1,I,K-1)+DIFF(1,I,K))/2.0
      DIFFAZ2=(DIFF(1,I,K)+DIFF(1,I,K+1))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      0X2=DIFFAX2*AX(1,K)*DX(1)
      0Y2=DIFFAY2*AY(1,K)*DY(1)
      0Z1=DIFFAZ1*AZ(1,1)*DZ(K-1)
      0Z2=DIFFAZ2*AZ(1,1)*DZ(K)
      DIFFCOEF=0X2+0Y2+0Z1+0Z2
C     COMPUTE ACETIC ACID FLOW DUE TO
DIFFUSION
      ADIFFX=0X2*C(2,I,K)
      ADIFFY=0Y2*C(1,2,K)
      ADIFFZ=0Z1*C(1,1,K-1)+0Z2*C(1,1,K+1)
      TOTDIFF=ADIFFX+ADIFFY+ADIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(1,I,K)/DT
C     COMPUTE NEW ACETIC ACID
CONCENTRATION
      AMP=TOTDIFF/COEFF+(1.0-DIFFCOEF/COEFF)*
C(1,I,K)
      C1(1,I,K)=AMP
C     SURFACE NODES  IMPOSED BOUNDARY
CONDITION
C     EXTERNAL EDGES (CONVECTION)
C     EDGES WITH INSULATION & CONVECTION
C     10  EDGE(1,I,MM,K)
C     11  EDGE(1,MM,J,K)
C     12  EDGE(1,I,1,K)
      C1(1,I,MM,K)=AC_BC
      C1(1,MM,J,K)=AC_BC
      C1(1,I,1,K)=AC_BC
      END DO
CCCCC
C     SLAB SURFACES (6)
      DO I=2,L
      JO I=2,M
C     PLANE OF SYMMETRY XY--(I,J,1)
C     COMPUTE AVERAGE DIFFUSIVITY
      DIFFAX1=(DIFF(I,J,1)+DIFF(I,J,1))/2.0
      DIFFAX2=(DIFF(I,J,1)+DIFF(I+1,J,1))/2.0
      DIFFAY1=(DIFF(I,J,1)+DIFF(I,J,1))/2.0
      DIFFAY2=(DIFF(I,J,1)+DIFF(I,J+1,1))/2.0
      DIFFAZ2=(DIFF(I,J,1)+DIFF(I,J,2))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
      0X1=DIFFAX1*AX(I,J)*DX(I-1)
      0X2=DIFFAX2*AX(I,J)*DX(I)
      0Y1=DIFFAY1*AY(I,J)*DY(J-1)
      0Y2=DIFFAY2*AY(I,J)*DY(J)
      0Z2=DIFFAZ2*AZ(I,J)*DZ(1)
      DIFFCOEF=0X1+0X2+0Y1+0Y2+0Z2
C     COMPUTE ACETIC ACID FLOW DUE TO
DIFFUSION
      ADIFFX=0X1*C(I-1,J,1)+0X2*C(I+1,J,1)
      ADIFFY=0Y1*C(I,J-1,1)+0Y2*C(I,J+1,1)
      ADIFFZ=0Z2*C(I,J,2)
      TOTDIFF=ADIFFX+ADIFFY+ADIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
      COEFF=DV(I,J,1)/DT
C     COMPUTE NEW ACETIC ACID
CONCENTRATION
      AMP=TOTDIFF/COEFF+(1.0-DIFFCOEF/COEFF)*
C(I,J,1)
      C1(I,J,1)=AMP
```

```
C     2---EXTERNAL SURFACE XY  (I,J,NN)
C     PRESCRIBED ACETIC ACID CONCENTRATION
        C1(I,J,NN)=AC_BC
        END DO
      END DO
CCCCC
      DO J=2,M
        DO K=2,N
C     3-PLANE OF SYMMETRY YZ  (1,J,K)
C     COMPUTE AVERAGE DIFFUSIVITY
        DIFFAX2=(DIFF(1,J,K)+DIFF(2,J,K))/2.0
        DIFFAY1=(DIFF(1,J-1,K)+DIFF(1,J,K))/2.0
        DIFFAY2=(DIFF(1,J,K)+DIFF(1,J+1,K))/2.0
        DIFFAZ1=(DIFF(1,J,K-1)+DIFF(1,J,K))/2.0
        DIFFAZ2=(DIFF(1,J,K)+DIFF(1,J,K+1))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
        BX2=DIFFAX2*AXG(K)/DX(1)
        BY1=DIFFAY1*AY(1,K)/DY(J-1)
        BY2=DIFFAY2*AY(1,K)/DY(J)
        BZ1=DIFFAZ1*AZ(1,J)/DZ(K-1)
        BZ2=DIFFAZ2*AZ(1,J)/DZ(K)
        DIFFCOEF=BX2+BY1+BY2+BZ1+BZ2
C     MOISTURE FLOW DUE TO DIFFUSION
        ADIFFX=BX2*C(2,J,K)
        ADIFFY=DY1*C(1,J-1,K)+BY2*C(1,J+1,K)
        ADIFFZ=BZ1*C(1,J,K-1)+BZ2*C(1,J,K+1)
        TOTDIFF=ADIFFX+ADIFFY+ADIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
        COFFF=DV(1,J,K)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
        AMP=TOTDIFF/COEFF*(1.0-DIFFCOEF/COEFF)*
C(1,J,K)
        C1(1,J,K)=AMP
C     4---EXTERNAL SURFACE YZ  (L,J,K)
C     PRESCRIBED ACETIC ACID CONCENTRATION
        C1(L,J,K)=AC_BC
        END DO
      END DO
CCCCC
      DO J=2,L
        DO K=2,N
C     5 PLANE OF SYMMETRY XZ  (I,1,K)
C     COMPUTE AVERAGE DIFFUSIVITY
        DIFFAX1=(DIFF(I-1,1,K)+DIFF(I,1,K))/2.0
        DIFFAX2=(DIFF(I,1,K)+DIFF(I+1,1,K))/2.0
        DIFFAY2=(DIFF(I,1,K)+DIFF(I,2,K))/2.0
        DIFFAZ1=(DIFF(I,1,K-1)+DIFF(I,1,K))/2.0
        DIFFAZ2=(DIFF(I,1,K)+DIFF(I,1,K+1))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
        BX1=DIFFAX1*AX(I,K)/DX(I-1)
        BX2=DIFFAX2*AX(I,K)/DX(I)
        BY2=DIFFAY2*AY(I,K)/DY(1)
        BZ1=DIFFAZ1*AZ(I,1)/DZ(K-1)
        BZ2=DIFFAZ2*AZ(I,1)/DZ(K)
        DIFFCOEF=BX1+BX2+BY2+BZ1+BZ2
C     MOISTURE FLOW DUE TO DIFFUSION
        ADIFFX=BX1*C(I-1,1,K)+BX2*C(I+1,1,K)
        ADIFFY=BY2*C(I,2,K)
        ADIFFZ=BZ1*C(I,1,K-1)+BZ2*C(I,1,K+1)
        TOTDIFF=ADIFFX+ADIFFY+ADIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
        COEFF=DV(I,1,K)/DT
C     COMPUTE NEW NODE MOISTURE CONTENT
        AMP=TOTDIFF/COEFF*(1.0-DIFFCOEF/COEFF)*
C(I,1,K)
        C1(I,1,K)=AMP
C     6---EXTERNAL SURFACE XZ  (I,M,K)
C     PRESCRIBED ACETIC ACID CONCENTRATION
        C1(I,M,K)=AC_BC
        END DO
      END DO
CCCCC
C     INTERIOR ELEMENT NODES
C     1  VOLUME XYZ  (I,J,K)
      DO I=2,L
        DO J=2,M
          DO K=2,N
C     COMPUTE AVERAGE DIFFUSIVITY
        DIFFAX1=(DIFF(I-1,J,K)+DIFF(I,J,K))/2.0
        DIFFAX2=(DIFF(I,J,K)+DIFF(I+1,J,K))/2.0
        DIFFAY1=(DIFF(I,J-1,K)+DIFF(I,J,K))/2.0
        DIFFAY2=(DIFF(I,J,K)+DIFF(I,J+1,K))/2.0
        DIFFAZ1=(DIFF(I,J,K-1)+DIFF(I,J,K))/2.0
        DIFFAZ2=(DIFF(I,J,K)+DIFF(I,J,K+1))/2.0
C     COMPUTE DIFFUSION RELATED
COEFFICIENTS
        BX1=DIFFAX1*AX(I,J,K)/DX(I-1)
        BX2=DIFFAX2*AX(I,J,K)/DX(I)
        BY1=DIFFAY1*AY(I,J,K)/DY(J-1)
        BY2=DIFFAY2*AY(I,J,K)/DY(J)
        BZ1=DIFFAZ1*AZ(I,J,K)/DZ(K-1)
        BZ2=DIFFAZ2*AZ(I,J,K)/DZ(K)
        DIFFCOEF=BX1+BX2+BY1+BY2+BZ1+BZ2
C     COMPUTE ACETIC ACID FLOW DUE TO
DIFFUSION
        ADIFFX=BX1*C(I-1,J,K)+BX2*C(I+1,J,K)
        ADIFFY=BY1*C(I,J-1,K)+BY2*C(I,J+1,K)
        AD FFZ=BZ1*C(I,J,K-1)+BZ2*C(I,J,K+1)
        TOTDIFF=ADIFFX+ADIFFY+ADIFFZ
C     COMPUTE TRANSIENT COEFFICIENT
        COEFF=DV(I,J,K)/DT
C     COMPUTE NEW ACETIC ACID
CONCENTRATION
        AMP=TOTDIFF/COEFF*(1.0-DIFFCOEF/COEFF)*
C(I,J,K)
        C1(I,J,K)=AMP
        END DO
      END DO
      RETURN
      END
C*****************************************************
      SUBROUTINE GRIDSH(XL,YM,ZN,L,M,N)
C*****************************************************
C     SUBROUTINE TO GENERATE SPACIAL GRID
C1  XL   LENGTH OF THE SLAB
C1  YM   WIDTH OF THE SLAB
C1  ZN   THICKNESS OF THE SLAB
C1  L    NO OF SPACE INTERVALS  X DIRECTION
C1  M    NO OF SPACE INTERVALS  Y DIRECTION
C1  N    NO OF SPACE INTERVALS  Z DIRECTION
C  O  X    NODE POSITION IN THE X DIRECTION
C  O  Y    NODE POSITION IN THE Y DIRECTION
C  O  Z    NODE POSITION IN THE Z DIRECTION
C  D  DX   SPACE INCREMENT IN THE X DIRECTION
C  D  DY   SPACE INCREMENT IN THE Y DIRECTION
C  D  DZ   SPACE INCREMENT IN THE Z DIRECTION
C  D  AX   ELEMENT AREA PERPEND. TO X AXIS
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C  D  AY   ELEMENT AREA PERPEND  TO Y AXIS
C  D  AZ   ELEMENT AREA PERPEND  TO Z AXIS
C  D  DY   ELEMENT VOLUME
C     I    INDEX FOR SPACE IN THE X DIRECTION
C     J    INDEX FOR SPACE IN THE Y DIRECTION
C     K.   INDEX FOR SPACE IN THE Z DIRECTION
C     DXX  DIST  BETWEEN AREAS ALONG X AXIS
C     DYY  DIST  BETWEEN AREAS ALONG Y AXIS
C     DZZ  DIST  BETWEEN AREAS ALONG Z AXIS
C*****************************************************
      COMMON /DIST/ DXX(15),DYY(15),DZZ(15)
      COMMON /SGRID/  X(15),Y(15),Z(15),DX(15),
     DY(15),DZ(15),AX(15,15),AY(15,15),AZ(15,15),
     DV(15,15,15)
C*****************************************************
C     GENERATE 3-D SPACE GRID
      LL=L+1
      MM=M+1
      NN=N+1
C     PROPORTIONS BETWEEN NODE POSITIONS
C     P1 & P2 ADD TO 1.0
      P1=0.25
      P2=0.75
C     COMPUTE SIZE OF SPACE SUBINTERVALS
C     NODE COORDINATES AND DISTANCES
C     BETWEEN ELEMENT VOLUMES
C     FOR NON-EQUALLY SPACED INTERIOR NODES
C        X DIRECTION
         DXX=XL/FLOAT(L)*4.0
         X(1)=0.0
         DX(1)=.5*DXX
         DXX(1)=P2*DX(1)
         DO I=2,L
          DX(I)=DXX*FLOAT(6-I+1)
          X(I)=X(I-1)+DX(I-1)
          DXX(I)=P1*DX(I-1)+P2*DX(I)
         END DO
         DX(LL)=.5
         X(LL)=X(L)+DX(L)
         DXX(LL)=P1*DX(L)
C        Y DIRECTION
         DDY=YM/FLOAT(M)/4.0
         Y(1)=0.0
         DY(1)=.5*DDY
         DYY(1)=P2*DY(1)
         DO J=2,M
          DV(J)=DDY*FLOAT(6-J+1)
          Y(J)=Y(J-1)+DV(J-1)
          DYY(J)=P1*DV(J-1)+P2*DV(J)
         END DO
         DY(MM)=0.0
         Y(MM)=Y(M)+DY(M)
         DYY(MM)=P1*DY(M)
C        Z DIRECTION
         DDZ=ZN/FLOAT(NN)*4.0
         Z(1)=0.0
         DZ(1)=.5*DDZ
         DZZ(1)=P2*DZ(1)
         DO K=2,N
          DZ(K)=DDZ*FLOAT(6-K+1)
          Z(K)=Z(K-1)+DZ(K-1)
          DZZ(K)=P1*DZ(K-1)+P2*DZ(K)
         END DO
         DZ(NN)=0.0
         Z(NN)=Z(N)+DZ(N)
         DZZ(NN)=P1*DZ(N)
CCCCC
C        CORNER ELEMENT VOLUMES (8)
C        1--CENTER NODE. ORIGIN OF COORD. SYSTEM
         (1 1 1)
            AX(1,1)=DYY(1)*DZZ(1)
            AY(1,1)=DXX(1)*DZZ(1)
            AZ(1,1)=DXX(1)*DYY(1)
            DV(1,1,1)=DXX(1)*DYY(1)*DZZ(1)
C        2--EXTERNAL NODE AT THE END OF X EDGE
         (LL,1,1)
            AY(LL,1)=DXX(LL)*DZZ(1)
            AZ(LL,1)=DXX(LL)*DYY(1)
            DV(LL,1,1)=DXX(LL)*DYY(1)*DZZ(1)
C        3--EXTERNAL NODE AT THE END OF Y EDGE
         (1,MM,1)
            AX(MM,1)=DYY(MM)*DZZ(1)
            AZ(1,MM)=DXX(1)*DYY(MM)
            DV(1,MM,1)=DXX(1)*DYY(MM)*DZZ(1)
C        4--EXTERNAL NODE AT THE END OF Z EDGE
         (1,1,NN)
            AX(1,NN)=DYY(1)*DZZ(NN)
            AY(1,NN)=DXX(1)*DZZ(NN)
            DV(1,1,NN)=DXX(1)*DYY(1)*DZZ(NN)
C        5--EXTERNAL NODE AT THE Y-Z INTERSECT
         (1,MM,NN)
            AX(MM,NN)=DYY(MM)*DZZ(NN)
            AY(1,NN)=DXX(1)*DZZ(NN)
            DV(1,MM,NN)=DXX(1)*DYY(MM)*DZZ(NN)
C        6--EXTERNAL NODE AT THE Y-Z INTERSECT
         (LL,MM,1)
            AY(LL,1)=DXX(LL)*DZZ(1)
            AZ(LL,MM)=DXX(LL)*DYY(MM)
            DV(LL,MM,1)=DXX(LL)*DYY(MM)*DZZ(1)
C        7--EXTERNAL NODE AT THE Z Y INTERSECT
         (LL,1,NN)
            AY(LL,NN)=DXX(LL)*DZZ(NN)
            DV(LL,1,NN)=DXX(LL)*DYY(1)*DZZ(NN)
C        8--EXTERNAL CORNER OPPOSITE TO CENTER.
         (LL,MM,NN)
            DV(LL,MM,NN)=DXX(LL)*DYY(MM)*DZZ(NN)
CCCCC
C        NODES ALONG THE SLAB EDGES (12)
C        ELEMENTS AT THE EDGES OF SYMMETRY
         (INSULATION)
C        1--X DIRECTION  DX FULL SIZE (1,1,1)
C        VOLUMES AT THE EXTERNAL EDGES
         (CONVECTION)
C        4--X DIRECTION  DX FULL SIZE (1,MM,NN)
C        VOLUMES AT EDGES W/ INSULATION &
         CONVECTION
C        7--X DIRECTION  DX FULL SIZE (1,MM 1)
            DO I=2,L
             AY(I,1)=DXX(I)*DZZ(1)
             AZ(I,1)=DXX(I)*DYY(1)
             DV(I,1,1)=DXX(I)*DYY(1)*DZZ(1)
             AY(I,NN)=DXX(I)*DZZ(NN)
             AZ(I,MM)=DXX(I)*DYY(MM)
             DV(I,MM,NN)=DXX(I)*DYY(MM)*DZZ(NN)
             DV(I,MM,1)=DXX(I)*DYY(MM)*DZZ(1)
             DV(I,1,NN)=DXX(I)*DYY(1)*DZZ(NN)
            END DO
C        2--Y DIRECTION  DY FULL SIZE (1,1,1)
C        5--Y DIRECTION  DY FULL SIZE (LL,1,NN)
C        8--Y DIRECTION  DY FULL SIZE (1,1,NN)
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      DO J=2,M
        AX(2,J)=DYY(J)*DZZ(1)
        AZ(1,J)=DXX(1)*DYY(J)
        DY(1,J)=DX(1)*DYY(J)*DZZ(1)
        AX(2,NN)=DYY(J)*DZZ(NN)
        AZ(LL-J)=DXX(LL)*DYY(J)
        DY(LL-1,NN)=DXX(LL)*DYY(J)*DZZ(NN)
        DY(LL,NN)=DXX(LL)*DYY(J)*DZZ(NN)
        DY(LL-1,1)=DXX(LL)*DYY(J)*DZZ(1)
      END DO
C     3  Z DIRECTION  DZ FULL SIZE (1 1,K)
C     8  Z DIRECTION  DZ FULL SIZE (LL,MM,K)
C     11 Z DIRECTION  DZ FULL SIZE (1,MM,K)
      DO K=2,N
        AZ(1,K)=DYY(1)*DZZ(K)
        AY(1,K)=DXX(1)*DZZ(K)
        DY(1 1,K)=DXX(1)*DYY(1)*DZZ(K)
        AX(MM,K)=DYY(MM)*DZZ(K)
        AY(1 1 K)=DXX(LL)*DZZ(K)
        DY(LL MM,K)=DXX(LL)*DYY(MM)*DZZ(K)
        DY(1,MM,K)=DXX(1)*DYY(MM)*DZZ(K)
        DY(LL-1 K)=DXX(LL)*DYY(1)*DZZ(K)
      END DO
CCCCC
C   8LAB SURFACES (6)
C     1  PLANE OF SYMMETRY XY  X & Y FULL SIZE
(1,J 1)
C     4  EXTERNAL SURFACE XY  X & Y FULL SIZE
(LJ,NN)
      DO I=2,L
        DO J=2,M
          AZ(I,J)=DXX(I)*DYY(J)
          DY(I,J 1)=DXX(I)*DYY(J)*DZZ(1)
          DY(I,J,NN)=DXX(I)*DYY(J)*DZZ(NN)
        END DO
      END DO
C     2  PLANE OF SYMMETRY YZ  Y & Z FULL SIZE
(1,J,K)
C     5  EXTERNAL SURFACE YZ  Y & Z FULL SIZE
(LL,J K)
      DO J=2,M
        DO k=2,N
          AX(J K)=DYY(J)*DZZ(K)
          DY(1,J K)=DXX(1)*DYY(J)*DZZ(K)
          DY(LL,J R)=DXX(LL)*DYY(J)*DZZ(K)
        END DO
      END DO
C     3  PLANE OF SYMMETRY XZ. X & Z FULL SIZE
(I 1 K)
C     6  EXTERNAL SURFACE XZ  X & Z FULL SIZE
(I,MM,K)
      DO I=2,L
        DO K=2,N
          AY(I,K)=DXX(I)*DZZ(K)
          DY(I 1,K)=DXX(I)*DYY(1)*DZZ(K)
          DY(I,MM,K)=DXX(I)*DYY(MM)*DZZ(K)
        END DO
      END DO
CCCCC
C   INTERIOR ELEMENT NODES
C     1  VOLUME XYZ. X, Y & Z FULL SIZE (I,J,K)
      DO I=2,L
        DO J=2,M
          DO K=2,N
            DY(I,J,K)=DXX(I)*DYY(J)*DZZ(K)
          END DO
        END DO
      END DO
      RETURN
      END
C*****************************************************
C   SUBROUTINE AIRPROP (TA,VA,X,Y,Z,A,RHO,
CPA,XIA,XMUA XD RE,XJH,XH,XKW)
C*****************************************************
C   SUBROUTINE FOR COMPUTING PHYSICAL
PROPERTIES OF AIR
C I  VA     AIR VELOCITY (M/S)
C I  TA     AIR TEMPERATURE (C)
C I  X,     SLAB SIZE IN THE X DIRECTION (M)
C I  Y      SLAB SIZE IN THE Y DIRECTION (M)
C I  Z      SLAB SIZE IN THE Z DIRECTION (M)
C  O RHO    AIR MASS DENSITY (KG/M3)
C  O XKA.   AIR THERMAL CONDUCT  (W/M.K)
C  O CPA.   AIR SPECIFIC HEAT CAPACITY (J/KG C)
C  O XMUA   AIR VISCOSITY (PA.S)
C  O XH.    HEAT TRANSFER COEFF (W/M2.C)
C  O XKW    MASS TRANSF COEFF  WATER
VAPOR (KG/M2.S)
C     VOL    VOLUME (M3)
C     XD     CHARACTERISTIC DIMENSION (M)
C     RE.    REYNOLDS NUMBER (L*V*RHO/MU)
C     PR     PRANDTH NUMBER ([MU*CP/K)
C     SCH.   SCHMIDT NUMBI R ([MU/RHO*DNFE)
C     XJD    COLBURN FACTOR FOR MASS TRANSFER
C     XJH    COLBURN FACTOR FOR HEAT TRANSFER
C*****************************************************
C   AIR VISCOSITY
      XMUA=(1 7328+0 00477*TA)*1 0E-5
C     AIR MASS DENSITY
      RHO=1 2573878-0 00343*TA
C     AIR SPECIFIC HEAT
      CPA= 1007 6882+( 0 05853*TA
C     THERMAL CONDUCTIVITY
      XKA=(0 02380+0 00005*TA
C     CARACTERISTIC DIMENSION
      A=2.0*(X*Y+X*Z+Y*Z)
      XD=A/(2*(X+Y))
C     KEYNOLDS NUMBER
      RE=XD*VA*RHO/XMUA
C     PRANTL NUMBER
      PR=0 7075
C     COLBURN FACTOR JH
      XJH=( 692*RE**(-0 488)
C     CONVECTIVE HEAT TRANSFER COEFFICIENT
      XH=XJH*RHO*VA*CPA/PR**(2/3 0)
C     COLBURN FACTOR JD
      XJD=XJH
C     SCHMIDT NUMBER
      SCH=0 745
C     CONVECTIVE MASS TRANSFER COEFFICIENT
      XKW=RHO*VA*XJD/SCH**(2 0/3 0)
      RETURN
      END
C*****************************************************
C   SUBROUTINE SIZE(W,X,Y,Z,A,VOL,XMASS,RHO)
C*****************************************************
C   SUBROUTINE TO COMPUTE SIZE AND SIZE
C   RELATED PROPERTIES CACAO BEANS AS A
C   FUNCTION OF TEMPERATURE AND MOISTURE
C I  W      MOISTURE CONTENT (DECIMAL, D.B.)
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```
C   O X     SLAB LENGTH   -X DIRECTION (M)
C   O Y     SLAB WIDTH    Y DIRECTION (M)
C   O Z     SLAB THICKNESS  Z DIRECTION (M)
C   O A     SLAB SURFACE AREA (M2)
C   O VOL   VOLUME OF THE SLAB (M3)
C   O XMASS  MASS OF THE SLAB (KG)
C   O RHO   MASS DENSITY (KG/M3)
C*****************************************************
C   COMPUTE SLAB GEOMETRIC PARAMETERS
X=(23.0582+1.1777*W-1.3059*W**2+1.6300*W**3)/
1000.0
Y=(13.1914+1.37394*W-3.8392*W**3+5.0689*W**3)/
1000.0
Z=(6.7264+0.8348*W+4.3170*W**2-2.6745*W**3)/
1000.0
C   SURFACE AREA
    A=2*(X*Y+X*Z+Y*Z)
C   MEAN VOLUME AND MASS
    VOL=X*Y*Z
    XMASS=(0.9703188+0.9356827*W)/1000.0
C   MEAN MASS DENSITY
    RHO=XMASS/VOL
    RETURN
    END
C*****************************************************
    SUBROUTINE MOISTAIR
(TA,TWA,RHA,TD,RHD,YW)
C*****************************************************
C   SUBROUTINE FOR COMPUTING PROPERTIES OF
MOIST AIR
C   AT A STATE SPECIFIED BY ITS DRY BULB AND
WET BULB
C   TEMPERATURES (K UNITS)
C 1  TA     DB TEMPERATURE OF AMBIENT AIR (C)
C 1  TWA    WB TEMPERATURE OF AMBIENT AIR (C)
C 1  TD     DB TEMPERATURE OF DRYING AIR (C)
C  O RHA    REL. HUMIDITY OF AMBIENT AIR (DEC)
C  O RHD    REL. HUMIDITY OF DRYING AIR(DEC)
C  O YW     MASS FRACTION (KG WATER
VAPOR/KG MOIST AIR)
C   TK.   TEMPERATURE (K)
C   T     TEMPERATURE (C)
C   PB    PRESSURE (KPA)
C   PA    PARTIAL PRESSURE OF DRY AIR (KPA)
C   PV    PARTIAL PRESS. OF WATER VAPOR (KPA)
C   PS    SAT. PRESSURE OF WATER VAPOR (KPA)
C   PSW   SAT PRESSURE VAPOR AT TWB (KPA)
C   PATM  ATMOSPHERIC PRESSURE (101.325 KPA)
C   XHFG  WATER LATENT HEAT OF VAP. (KJ/KG)
C   W     HUMID. RATIO (KG VAPOR/KG DRY AIR)
C   R.    GAS CONSTANT (8314.41 M3 KPA/KG K)
C   XMA   MOL. WEIGHT OF DRY AIR (28.9645)
C   XMV   MOL. WEIGHT OF WATER (18.01534)
C   XN    RATIO OF MOLECULAR WEIGHT OF
C         WATER TO MOL. WEIGHT OF DRY AIR
C*****************************************************
    PARAMETER(R=8314.41  PATM=101.325)
    PARAMETER(XMA=28.9645  XMV=18.01534)
    PARAMETER(TK=273.16)
    PARAMETER(CPA=1.0056  CPV=1.8460)
    PARAMETER(RA=R/XMA, RV=R/XMV)
    PARAMETER(XN=XMV/XMA)
C*****************************************************
C   STATEMENT FUNCTIONS
C   TEMPERATURE IN DEGREE C TO K
    TK(T)=T+TK.0
C   HUMIDITY RATIO
    HR(P)=XN*P/(PATM-P)
C   MASS FRACTION
    XMF(H)=H/(1.0+H)
C   SPECIFIC VOLUME
    VOL(R,T,P)=RR*TK(T)/P
C   SPECIFIC HEAT
    CP(X)=CPA+HR(X)*CPV
C   LATENT HEAT OF VAPORIZATION
    XLFG(T)=2500.80-2.3668*T
C   SATURATION VAPOR PRESSURE
(WEXLER-GRELNSPAN EQ)
    PSAT(T)=EXP(.7511.52/TK(T)+89.63121+
0.02398*TK(T)
     1.165455E-05*TK(T)**2-1.2810336E-08*TK(T)**3
    +2.0998408E 11*TK(T)**4-12.150799*LOG(TK(T))
C   COMPUTATION OF AMBIENT AIR PROPERTIES
C   SAT. VAPOR PRESSURE AT DRY TEMPERATURE
    PSA=PSAT(TA)
C   SAT. VAPOR PRESSURE AT WB TEMPERATURE
    PSW=PSAT(TWA)
C   PARTIAL PRESSURE OF WATER VAPOR
    WW=HR(PSW)
    A=(XN*CP(PSW))/(XN+WW)**3*XLFG(TWA))
    PV=PSW/A*PATM/(TA-TWA)
C   HUMIDITY RATIO
    W=HR(PV)
C   MASS FRACTION
    YW=XMF(W)
C   RELATIVE HUMIDITY
    RHA=PV/PSA
C   COMPUTATION OF DRYING AIR PROPERTIES
C   SAT. VAPOR PRESSURE AT DR TEMPERATURE
    PSD=PSAT(TD)
    RHD=PV/PSD
    RETURN
    END
C*****************************************************
    SUBROUTINE DIFFUS(T,W,DEFF)
C*****************************************************
C   SUBROUTINE TO COMPUTE EFF. DIFFUS. OF
C   THE PRODUCT AS A FUNCTION OF ITS
C   TEMPERATURE AND MOISTURE  D=D(W,T)
C 1  T     TEMPERATURE (K--KELVIN, C--CELCIUS)
C 1  W     MOISTURE CONTENT (DEC/MAL. DB)
C  O DEFF   EFFECTIVE DIFFUSIVITY (M2/S)
C*****************************************************
C   COMPUTE EFFECTIVE DIFFUSIVITY D=D(W,T)
    TK=T+273.16
C   VARIABLE DIFFUSIVITY
    A=9.142E-05
    B=3.072
    C=16.522
    D=-9.133
    E=-4565.6
    DEFF=A*EXP(B*W+C*W**2+D*W**3+E/TK)
    RETURN
    END
C*****************************************************
    SUBROUTINE AVERAGE
(L,MN,TIMI,DUR,AVGC,AVGW,AVGT)
C*****************************************************
C   COMPUTE AVERAGE OVER A 3-D DOMAIN
C 1  L      ARRAY DIMENSION 1
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C     M       ARRAY DIMENSION 2
C     N       ARRAY DIMENSION 3
C     TIME    CURRENT TIME
C     DUR     PROCESS DURATION
C     AVGC    ACETIC ACID AVERAGE
C     AVGW    MOISTURE AVERAGE
C     AVGT    TEMPERATURE AVERAGE
C     CA      ACETIC ACID CONCENTRATION
C     W       MOISTURE CONTENT
C     T       TEMPERATURE
C     WT      WEIGHT
C*************************************************
      COMMON /TEMP/  T(15 15 15) T1(15 15 15)
      COMMON /MOIST/  W(15 15 15),W1(15 15 15)
      COMMON /ACID/  C1(15 15 15) C(15 15 15)
      COMMON /SPGRAV/ X(15),Y(15),Z(15),DX(15),
     DY(15) DY1(15),AX(15 15),AY(15 15),AZ(15,15)
     DV(15 15 15)
C*************************************************
C     OPEN FILE AND WRITE TABLE HEADINGS
      DATA=DUR
     OPEN(UNIT=2,FILE='DRYSS20 PRN',ACCESS='APPEN
     D',STATUS='UNKNOWN')
       IF(TIME EQ 0.0) THEN
         WRITE(2,*)'DRYING OF FULLY EXPOSED
     CACAO BEANS'
         WRITE(2,FMT='(A)')' SPACE GRID
         WRITE(2,*)A,(3)' # OF NODES X DIRECTION  L
         WRITE(2,*)A,(3)' # OF NODES Y DIREC TION  M
         WRITE(2,*)A,(3)' # OF NODES Z DIRECTION  N
         WRITE(2,*)A)' TIME   TAVG   WAVG   CAVG'
       ELSE
       ENDIF
C     COMPUTE SUMS
      SUMC=0.0
      SUMW=0.0
      SUMT=0.0
      SUMWT=0.0
C     COMPUTE DENSITY OF DRY BONE MATERIAL
     WW=0.0
      CALL SIZE(WW,X,Y,Z,A,VOL,XMASS,RHOD)
C     COMPUTE SUMS
        DO I=1,L
          DO J=1,M
            DO K=1,N
              WT=DV(I,J,K)*RHOD
              SUMC=SUMC+C1(I,J,K)*WT
              SUMW=SUMW+W1(I,J,K)*WT
              SUMT=SUMT+T1(I,J,K)*WT
              SUMWT=SUMWT+WT
            END DO
          END DO
        END DO
C     COMPUTE AVERAGE
      AVGC=SUMC/SUMWT
      AVGW=SUMW/SUMWT
      AVGT=SUMT/SUMWT
C     OUTPUT RESULTS TO FILE
     WRITE(2,'(F8.1,F10.2,2F10.6)')TIME,AVGT,AVGW,AVG
      CLOSE(UNIT=2)
      RETURN
      END
C*************************************************
      SUBROUTINE HFND_MODIFY(AW,W)
C*************************************************
C     SUBROUTINE TO COMPUTE WATER ACTIVITY C
C     EMC EQUATION HENDERSONS MODIFIED
C     T       TEMPERATURE(C)
C     WE      EQ MOISTURE CONTENT (DEC  DB)
C     AW      WATER ACTIVITY (DECIMAL)
C*************************************************
      PARAMETER
     (A=-6.414E-2,B=10.43,C=4.688E8,D=-1.714)
C*************************************************
C     COMPUTE WATER ACTIVITY AW=F(T W)
      TK=T+273.15
      V1=A*TK**B
      V2=W**(C*(TK**D))
      AW=1.0+EXP(V1*V2)
      RETURN
      END
C*************************************************
      SURRDUTINE VAPOR_FRACTION(TD AW YW)
C*************************************************
C     SURROUNTE TO COMPUTE MASS FRACTION OF
C     WATER VAPOR IN AIR
C     TD    DRY BULB TEMPERATURE (C)
C     AW    WATER ACTIVITY (DECIMAL)
C     YW    MASS FRACTION (KG WATER
     VAPOR/KG MOIST AIR)
C     TK    TEMPERATURE (K)
C     P     PRESSURE (KPA)
C     PA    PARTIAL PRESSURE OF DRY AIR (KPA)
C     PV    PARTIAL PRESS OF WATER VAPOR (KPA)
C     PS    SAT PRESSURE OF WATER VAPOR (KPA)
C     PATM  ATMOSPHERIC PRESSURE (101.325 KPA)
C     W     H. RATIO (KG WATER VAPOR/KG DRY AIR)
C     R     DAS CONSTANT (8314.4 [ M3 KPA/KG K)
C     XMA   MOL. WEIGHT OF DRY AIR (28.9645)
C     XMV   MOL. WEIGHT OF WATER (18.01534)
C     XN    RATIO OF MOLECULAR WEIGHT OF
C        WATER TO MOLECULAR WEIGHT OF DRY AIR
C*************************************************
      PARAMETER(R=8314.41 PATM=101.325)
      PARAMETER(XMA=28.9645 XMV=18.01534)
      PARAMETER(TK=T+273.15)
      PARAMETER(RA=R/XMA, RV=R/XMV)
      PARAMETER(XN=XMV/XMA)
C*************************************************
C     STATEMENT FUNCTIONS
C     TEMPERATURE IN DEGREE C TO K
     TK(T)=T+TK0
C     HUMIDITY RATIO
      HR(P)=XN*P/(PATM-P)
C     MASS FRACTION
      XM(H)=H/(1.0+H)
C     SATURATION VAPOR PRESSURE
     (WEXLER-GREENSPAN EQ)
      PSAT(T)=EXP(-5811.52/TK(T)+89.63121+
     0.02395897*TK(T)
     1-1.6545151E-05*TK(T)**2-1.2981036E-08*TK(T)**3
     +2.0998465E-11*TK(T)**4-12.150924*LOG(TK(T)))
C     COMPUTATION OF AMBIENT AIR PROPERTIES
C     SATURATION VAPOR PRESSURE AT DRY BULB
     TEMPERATURE
      PS=PSAT(TD)
C     PARTIAL PRESSURE OF WATER VAPOR
      PV=AW*PS
C     HUMIDITY RATIO
      W=HR(PV)
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C   MASS (HUMIDITY) FRACTION
    YW=XMF(W)
    RETURN
    END
C*********************************************************
    SUBROUTINE THERMAL(T,W,CP,XK)
C*********************************************************
C   SUBROUTINE TO COMPUTE THE THERMAL
C   PROPERTIES OF CACAO AS A FUNCTION OF
C   TEMPERATURE AND/OR MOISTURE
C I  T      TEMPERATURE (K,  KELVIN, C  CELCIUS)
C I  W      MOISTURE CONTENT (DB)
C  O CP     SPECIFIC HEAT CAPACITY (J/KG.C)
C  O XK     THERMAL CONDUCTIVITY (W/M.C)
C*********************************************************
    TC=T
C   SPECIFIC HEAT CAPACITY (SASSERON, 1984)
    CP=(3.09+1.82*W ) 58*W**2)*1000.0
C   THERMAL CONDUCTIVITY (SASSERON  1984)
    XK=0.180+0.266*W-7.81E-4*TC
    RETURN
    END
C*********************************************************
    SUBROUTINE XLHEAT(T,W,AW,XL)
C*********************************************************
C   SUBROUTINE TO COMPUTE LATENT HEAT OF
C   VAPORIZATION
C   EMC EQUATION
C        DAY & NELSON'S HENDERSON MODIFIED
C I  T      TEMPERATURE (K—KELVIN  C   CELCIUS)
C I  W      MOISTURE CONTENT (DECIMAL,  DB)
C  O XL     LATENT HEAT OF VAPORIZATION (J/KG)
C  O AW     WATER ACTIVITY (DEC IMAL)
C   XL=     WATER LAT HT OF VAPORIZATION (J/KG)
C   XLW     WATER SORPTION HEAT (J/KG)
C   R,      GAS CONSTANT [8314.41 J/KG.K)
C           GAS CONSTANT FOR WATER VAPOR
C   XMV     MOL. WEIGHT OF WATER (18.01534)
C*********************************************************
    PARAMETER
(A=-4.414E-24,B=10.43,C=4.588E4,D=-1.714)
    PARAMETER (R=461.5186)
C*********************************************************
C   COMPUTE WATER ACTIVITY AW=F(W,T,C)
C   MODIFIED HENDERSON EQUATION
    TK=T+273.15
    Y1=A*TK**B
    Y2=-W**(C*TK**D)
    AW=1.0-EXP(Y1*Y2)
C   SATURATION VAPOR PRESSURE
(WEXLER-GREENSPAN EQN )
    TK=T+273.15
DXLNPS=-7511.52/TK**2+0.02390907-2*1.1656
551E-05*Tk
 3*1.2810336E-08*TK**2+4*2.0998485E-11*TK**3
-12.150799/TK
C   LAT HEAT OF VAPORIZATION OF PURE WATER
    XL=R*TK**2*DXLNPS
C   HEAT OF SORPTION
    Y12=Y1*Y2
    Z1=EXP(Y12)
    Z2=1.0+Z1
    Z3=Z1/Z2
    Z4=Z3*Y12*TK*(B+C*D*LOG(W)*TK**D)
    XLW=R*Z4
    XL=XL0+XLW
    RETURN
    END
C*********************************************************
    SUBROUTINE DRY_SPLINE(XI,YI,NN,TINT,Y2I)
C*********************************************************
    REAL XI(NN),YI(NN),Y2I(100)
C*********************************************************
    YP1=2.e30
    YPN=2.e30
    KX=0.0
    XTOT=XI(NN)
    DX=TINT/10
C   COMPUTE SECOND DERIVATIVES OF THE
INTERPOLATING
C     FUNCTION AT THE TABULATED POINTS Xi
C   USES SUBROUTINE SPLINE   NUMERICAS
RECIPES (1992)
    CALL SPLINE(XI,YI,NN,YP1,YPN,Y2)
    DO WHILE(XX.LE.XTOT)
C   COMPUTE INTERPOLATED VALUE Y FOR A
GIVEN X
C     USES SUBROUTINE SPLINT   NUMERICAL
RECIPES (1992)
      CALL SPLINT(XI,YI,Y2,NN,XX,YY)
C   COMPUTE FIRST DERIVATIVE AT THE GIVEN X
C     USES FUNCTION DFRIDR  NUMERICAL
RECIPES (1992)
C       MODIFIED AND TRANSFORMED INTO A
SUBROUTINE
      CALL DFDX(XI,YI,Y2,NN,XX,DX,ERR,DYDX)
C     INCREMENT X
      XX=XX+TINT
    END DO     ! end do while
    RETURN
    END
C*********************************************************
C*********************************************************
    SUBROUTINE DFDX(XI,YI,Y2,NN,x,h,err,DFRIDR)
C   NUMERICAL DERIVATIVE (MODIFIED)
C (C) Copr. 1986-92 Numerical Recipes Software
(MODIFIED)
    SUBROUTINE spline(x,y,n,yp1,ypn,y2)
C   CUBIC SPLINE
C (C) Copr. 1986-92 Numerical Recipes Software
    SUBROUTINE splint(xa,ya,y2a,n,x,y)
C   NUMERICAL INTERPOLATION
C (C) Copr. 1986-92 Numerical Recipes Software
    SUBROUTINE locate(xx,n,x,j)
C (C) Copr. 1986-92 Numerical Recipes Software
%is=$21n  &,))
C*********************************************************
C*********************************************************
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SAMPLE OF INPUT FILE TEST 02

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DRYING, MEAN AMBIENT AND WET BULB TEMPERATURES (C),
AND AIR VELOCITY (M/S)
READ(UNIT=1,FMT='(///,4F10.2)')TD,TA,TW,VA
   60 46    29 23    25 55    2 55
PRODUCT TEMPERATURE (C)  MOISTURE AND ACID CONTENTS (DEC, DB)
READ(UNIT=1,FMT='(//,F10 2 3F10 4)')T0,W0,C0,AC0
   26.20   1 1035   0 0175   0 0000
PROCESS DURATION (S) AND TIME INCREMENT (S)
READ(UNIT=1,FMT='(//,2F10.2)')DUR,DT
 180000 00     0 25
NUMBER OF SPACE SUBINTERVALS (X, Y AND Z DIRECTIONS)
READ(UNIT=1 FMT='(//,315)')LX,MY NZ
   5   5   5
PRINTING STEP IN TIME (S) AND SPACE (UNITS) - X, Y  Z DIRECTIONS
READ(UNIT=1,FMT='(//,F10 2 315)')PTIME,LPX,MPY,NPZ
   120 00   3   3   3
0          1 1035   26.2     24 4
600        0 8855
900        0 8141   26.2     24 4
1800       0 692    26 7     24 9
3600       0 5699   26 7     25 3
5400       0 4985   29 0     26 5
7200       0 4478   29 4     26 0
9000       0 4085   30 5     25 5
10800      0 3764   31.5     25.5
12600      0 3493   31 5     25 1
14400      0 3257   31.5     25.5
16200      0 305    31 5     26 0
19800      0 2696   32 0     26 0
23400      0 2402   32 0     26 2
27000      0 215    31 6     25.5
30600      0 193    30 5     25 2
34200      0 1734   29.5     25.5
41400      0 1397   28 0     25 6
45000      0 125    27.9     26.5
48600      0 1115   27 1     25 5
52200      0 0989   27 0     25 4
55800      0 0871   27 0     25 1
59400      0 0812   26 8     25.3
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I certify that I have read this study and that in my opinion it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a thesis for the degree of Doctor of Philosophy

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